

Nonequilibrium Dynamics in Low Dimensional Systems

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Abstract

In these lectures we give an overview of nonequilibrium stochastic systems. In particular we discuss in detail two models, the asymmetric exclusion process and a ballistic reaction model, that illustrate many general features of nonequilibrium dynamics: for example coarsening dynamics and nonequilibrium phase transitions. As a secondary theme we shall show how a common mathematical structure, the q -deformed harmonic oscillator algebra, serves to furnish exact results for both systems. Thus the lectures also serve as a gentle introduction to things q -deformed.

Key words: Nonequilibrium Dynamics, Stochastic Processes, Phase Transition, Asymmetric Exclusion Process, Reaction Kinetics

PACS: 02.50.-r, 05.40.-a, 05.70.Fh

1 Introduction

In these lectures we explore the subject of nonequilibrium dynamics. Before getting into any kind of detail let us first establish what we mean by a nonequilibrium system. This is best done by taking stock of our understanding of an equilibrium system. Consider the Canonical (Boltzmann) distribution for a systems with configurations labelled \mathcal{C} each with energy $E(\mathcal{C})$:

$$P(\mathcal{C}) = \frac{\exp(-\beta E(\mathcal{C}))}{Z} \quad (1)$$

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where $\beta = 1/kT$. The task is to calculate the partition function

$$Z = \sum_{\mathcal{C}} \exp(-\beta E(\mathcal{C})) , \quad (2)$$

from which all thermodynamic properties, in principle, can be computed. The distribution (1) applies to systems in thermal equilibrium *i.e.* free to exchange energy with an environment at temperature T . It can easily be generalised to systems free to exchange particles, volume etc but it always relies on the concept of the system being at equilibrium with its environment.

If one were interested in dynamics, for example to simulate the model on a computer, one might choose transition rates between configurations to satisfy

$$W(\mathcal{C}' \rightarrow \mathcal{C})e^{-\beta E(\mathcal{C}')} = W(\mathcal{C} \rightarrow \mathcal{C}')e^{-\beta E(\mathcal{C})} \quad (3)$$

where $W(\mathcal{C}' \rightarrow \mathcal{C})$ is the transition rate from configuration \mathcal{C}' to \mathcal{C} . Condition (3) is known as detailed balance and guarantees (under the assumption of ergodicity to be discussed below) that starting from some nonequilibrium initial condition the system will eventually reach the steady state of thermal equilibrium given by (1). We will discuss further this dynamical relaxation process and the properties of the steady state endowed by the detailed balance condition in Section 3. For the moment we note that a system relaxing to thermal equilibrium is one realisation of a nonequilibrium system. In recent years such relaxation dynamics have been of special interest, for example, in the study of glassy dynamics whereby, on timescales realisable in experiment (or simulation), the system never reaches the equilibrium state and it is a very slowly evolving nonequilibrium state that is observed. This is sometimes referred to as ‘off-equilibrium’ dynamics. Also let us mention the field of domain growth whereby an initially disordered state is quenched (reduced to a temperature below the critical temperature for the ordered phase) and relaxes to an ordered state through a process of coarsening of domains. The interesting physics lies in the scaling regime of the coarsening process which is observed before the equilibrium (ordered) state is reached.

The other meaning of nonequilibrium refers to a system that reaches a steady state, but not a steady state of thermal equilibrium. Examples of such nonequilibrium steady states are given by driven systems with open boundaries where a mass current is driven through the system. Thus the system is driven by its environment rather than being in thermal equilibrium with its environment.

A pragmatic definition of a nonequilibrium system that encompasses all of the scenarios above is as a model defined by its dynamics rather than any energy function *i.e.* the configurations of the model are sampled through a local stochastic dynamics which *a priori* does not have to obey detailed balance.

1.1 *Structure of these notes*

These notes broadly follow the four lectures given at the summer school. In addition a tutorial class was held to explore points left as exercises in the lectures. In the present notes these exercises are included in a self-contained form that should allow the reader to work through them without getting stuck or else leave them for another time and continue with the main text. The notes are structured as follows: in section 2 we give an overview of two simple models that we are mainly concerned with in these lectures. In section 3 we then set out the general theory of the type of stochastic model we are interested in and point out the technical difficulties in calculating dynamical or even steady-state properties. Section 4 is an interlude in which we introduce, in a self-contained way, a mathematical tool—the q -deformed harmonic oscillator—that will prove itself of use in the final two sections. In Section 5 we present the solution of the partially asymmetric exclusion process and amongst other things how the phase diagram (Figure 3) is generalised. In Section 6 we discuss the exact solution of a stochastic ballistic annihilation and coalescence model.

2 Two simple models

In this work we will focus on two exemplars of nonequilibrium systems: the partially asymmetric exclusion process and a particle reaction model. These models have been well studied over the years and a large body of knowledge has been built up [1]. We introduce the models at this point but will come back to these models in more detail in Sections 5 and 6 in which we summarise some recent analytical progress.

2.1 *Asymmetric exclusion process*

2.1.1 *Model definition*

The asymmetric simple exclusion process (ASEP) is a very simple driven lattice gas with a hard core exclusion interaction [2]. Consider M particles on a one-dimensional lattice of length N say. At each site of the lattice there is either one particle or an empty site (to be referred to as a vacancy or hole)—there is no multiple occupancy.

The dynamics are defined as follows: during each time interval ΔT each particle has probability ΔT of attempting a jump to its right and probability $q\Delta T$ of attempting a jump to its left; a jump can only succeed if the target site is

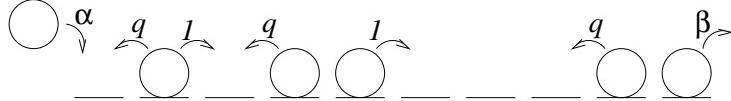


Fig. 1. Dynamics of the partially asymmetric exclusion process with open boundaries.

empty.

In this work will be concerned with the case $\Delta T = dt \rightarrow 0$ so that we obtain continuous time dynamics with particles attempting hops to the right with rate 1 and hops to the left with rate q . In this limit no two particles will jump at the same time. The other limit of $\Delta T = 1$ would correspond to fully parallel dynamics where all particles attempt hops at the same time. This type of dynamics is employed (for $q = 0$) in traffic flow modelling (see Schadschneider this volume).

To complete the specification of the dynamics we have to fix the boundary conditions. It turns out these are of great significance. The following types of boundary conditions have been considered:

Periodic In this case we identify site $N + 1$ with site 1. The particles then hop around a ring and the number of particles is conserved.

Open boundaries In this case particles attempt to hop into site 1 with rate α . A particle at site N leaves the lattice with rate β . Thus the number of particles is not conserved at the boundaries. One can also understand these boundary conditions in terms of a site 0 being a reservoir of particles with fixed density α and site $N + 1$ being a reservoir with fixed density $1 - \beta$. We shall primarily be concerned with these boundary conditions because, as first pointed out by Krug [3], they can induce phase transitions. The dynamics is illustrated in Figure 1.

Closed boundaries In this case the boundaries act as reflecting walls and particles can not enter or leave the lattice. Thus one has a zero current of particles in the steady state and the system obeys detailed balance. We shall not be interested in this case.

Infinite system Finally we could consider our lattice of size N as a finite segment of an infinite system.

2.1.2 Density and current in the ASEP

The macroscopic properties of the ASEP in which we are interested are the steady-state current (flux of particles across the lattice) and density profile (average occupancy of a lattice site). These can be expressed in terms of the binary variables $\{\tau_i\}$, where $\tau_i = 1$ if site i is occupied by a particle and $\tau_i = 0$ if site i is empty, and which together completely specify a microscopic configuration of the system. Then, the density at site i is defined as $\langle \tau_i(t) \rangle$

where the angular brackets denote an average over all histories of the stochastic dynamics. One can think of this average as being an average over an ensemble of systems all starting from the same initial configuration at time 0.

Let us consider for the moment the totally asymmetric dynamics $q = 0$ (*i.e.* no backward particle hops are permitted). One can use the ‘indicator’ variables $\{\tau_i\}$ intuitively to write down an equation for the evolution of the density. For example, if we choose a non-boundary site (so that we can avoid prescribing any particular boundary conditions) we obtain

$$\frac{d\langle \tau_i \rangle}{dt} = \langle \tau_{i-1}(1 - \tau_i) \rangle - \langle \tau_i(1 - \tau_{i+1}) \rangle. \quad (4)$$

Note that $\langle \tau_{i-1}(1 - \tau_i) \rangle$ gives the probability that site $i - 1$ is occupied and site i is empty. Thus, since particles hop forward with rate 1, first term on the right hand side gives the rate at which particles enter site i and the second term gives the rate at which they leave site i .

If one needs more convincing of the argument used to obtain (4) consider what happens at site i in an infinitesimal interval dt :

$$\tau_i(t + dt) = \begin{cases} \tau_i(t) & \text{with probability } 1 - 2dt \\ \tau_i(t) + [1 - \tau_i(t)] \tau_{i-1}(t) & \text{with probability } dt \\ \tau_i(t) \tau_{i+1}(t) & \text{with probability } dt \end{cases}. \quad (5)$$

The first equation comes from the fact that with probability $1 - 2dt$ (dropping terms of $O(dt^2)$), neither of the sites $i - 1$ or i is updated and therefore τ_i remains unchanged. The second and the third equations correspond to updating sites $i - 1$ and i respectively. If one averages (5) over the events which may occur between t and $t + dt$ and all histories up to time t one obtains (4).

The same kind of reasoning allows one to write down straight away an equation for the evolution of $\langle \tau_i \tau_{i+1} \rangle$.

$$\frac{d\langle \tau_i \tau_{i+1} \rangle}{dt} = \langle \tau_{i-1}(1 - \tau_i) \tau_{i+1} \rangle - \langle \tau_i \tau_{i+1}(1 - \tau_{i+2}) \rangle \quad (6)$$

or for any other correlation function $\langle \tau_i \tau_j \dots \rangle$. These equations are exact and give in principle the time evolution of any correlation function. However, the evolution (4) of $\langle \tau_i \rangle$ requires the knowledge of $\langle \tau_i \tau_{i+1} \rangle$ which itself (6) requires the knowledge of $\langle \tau_{i-1} \tau_{i+1} \rangle$ and $\langle \tau_{i-1} \tau_i \tau_{i+1} \rangle$ so that the problem is intrinsically an N -body problem in the sense that the calculation of any correlation function requires the knowledge of all the others. This is a situation quite common in equilibrium statistical mechanics where, although one can write relationships between different correlation functions, there is an infinite hierarchy of equations which in general makes the problem intractable.

For the case of open boundary conditions the number of particles in the system is not conserved. The evolution equations (4-6) are then valid everywhere in the bulk but they are modified at the boundary sites. For example (4) becomes

$$\frac{d\langle\tau_1\rangle}{dt} = \alpha\langle(1 - \tau_1)\rangle - \langle\tau_1(1 - \tau_2)\rangle \quad (7)$$

$$\frac{d\langle\tau_N\rangle}{dt} = \langle\tau_{N-1}(1 - \tau_N)\rangle - \beta\langle\tau_N\rangle. \quad (8)$$

In the steady state, where the time derivatives of correlation functions are zero, (4,7,8) can be rewritten as a conserved current J

$$J = \alpha\langle(1 - \tau_1)\rangle = \langle\tau_1(1 - \tau_2)\rangle = \cdots \langle\tau_{i-1}(1 - \tau_i)\rangle = \cdots \langle\tau_{N-1}(1 - \tau_N)\rangle = \beta\langle\tau_N\rangle. \quad (9)$$

These equations simply express that for the density to be stationary one must have the current into any site equal to the current out of that site. For example, $\alpha\langle(1 - \tau_1)\rangle$ is the probability that the leftmost site is empty multiplied by the rate at which particles are inserted onto it, and hence yields the current of particles entering the system. Similarly $\beta\langle\tau_N\rangle$ is the rate at which particles leave the system.

2.1.3 Applications of the ASEP

To motivate the study of this model let us consider a few applications. First we may consider the ASEP as a very simplistic model of traffic flow with no overtaking (more realistic generalisations are discussed by Schadschneider, this volume). Joining many open boundary systems together into a network forms a very simple model for city traffic. Such a network appears to represent faithfully real traffic phenomena such as jamming [4].

A major motivation for the study of the ASEP is its connection to interface dynamics and hence to the KPZ equation (noisy Burgers' equation). The KPZ equation is a stochastic non-linear partial differential equation that is central to much of modern statistical physics. In these lectures we do not have time to develop the theory of the KPZ equation, rather we refer the reader to [5]. Here we just make clear the connection to a particular interface growth model.

The asymmetric exclusion model may be mapped exactly onto a model of a growing interface in $(1+1)$ dimensions [6] as shown in Figure 2. The mapping is obtained by associating to each configuration $\{\tau_i\}$ of the particles a configuration of an interface: a particle at a site corresponds to a downwards step of the interface height of one unit whereas a hole corresponds to an upward

step of one unit. The heights of the interface are thus defined by

$$h_{i+1} - h_i = 1 - 2\tau_i . \quad (10)$$

The dynamics of the asymmetric exclusion process in which a particle at site $i - 1$ may interchange position with a neighbouring hole at site i , corresponds to a growth at a site i which is a minimum of the interface height *i.e.* if $h_i(t) = h_{i-1}(t) - 1 = h_{i+1}(t) - 1$ then

$$h_i \rightarrow h_i(t) + 2 \quad \text{with rate } 1 . \quad (11)$$

A growth event turns a minimum of the surface height into a maximum thus the ASEP maps onto what is known as a single-step growth model [6] meaning that the difference in heights of two neighbouring positions on the interface is always of magnitude one unit. Since whenever a particle hops forward the interface height increases by two units, the velocity v at which the interface grows is related to J the current in the asymmetric exclusion process by

$$v = 2J . \quad (12)$$

Periodic boundary conditions for the particle problem with M particles and $N - M$ holes correspond to an interface satisfying $h_{i+N} = h_i + N - 2M$, *i.e.* to helical boundary conditions with an average slope $1 - 2M/N$. The case of open boundary conditions corresponds to special growth rules at the boundaries. Because of this equivalence, several results obtained for the asymmetric exclusion process can be translated into exactly computable properties of the growing interface.

One can also go on to list further applications [7]. Indeed early applications concerned biophysical problems such as single-filing constraint in transport across membranes [8] and the kinetics of biopolymerisation [9].

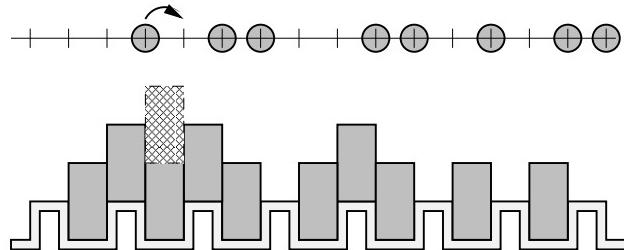


Fig. 2. The single-step growth model and its mapping onto the asymmetric exclusion process with $q = 0$. Note that the addition of a new particle to the surface (shown light-shaded) corresponds to the rightward hop of a particle in the ASEP.

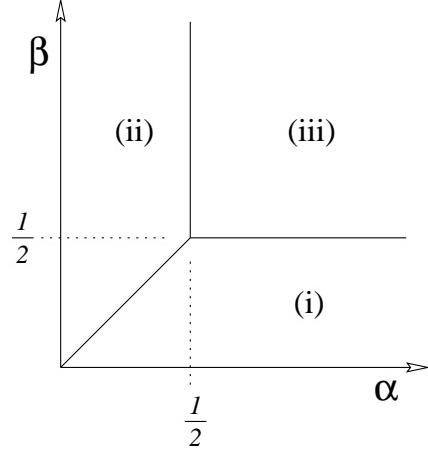


Fig. 3. Phase diagram for the totally asymmetric exclusion process ($q = 0$).

2.1.4 Phase diagram for $q = 0$

Let us now discuss some interesting results that have been derived over the last decade for the open boundary system [10,11]. For the moment we present them without proof, although we shall recover some of them in the analysis of later sections. In Figure 3 we present the phase diagram (corresponding to the limit $N \rightarrow \infty$) for the totally asymmetric exclusion process *i.e.* when $q = 0$ as predicted within a mean-field approximation [9,12]. It should be noted that we consider the steady state in the limit $N \rightarrow \infty$, thus it is implicit that we have taken the limit $t \rightarrow \infty$ first. Note there are three phases—by phase it is meant a region in the phase diagram where the current has the same analytic form; phase boundaries divide regions where the current J and bulk density ρ (defined as the mean occupancy of a site near the centre of the lattice as $N \rightarrow \infty$) have different forms:

(i) *High density phase* For $\beta < \frac{1}{2}$ and $\alpha > \beta$,

$$J = \beta(1 - \beta) \quad \rho = 1 - \beta \quad (13)$$

(ii) *Low density phase* For $\alpha < \frac{1}{2}$ and $\beta > \alpha$,

$$J = \alpha(1 - \alpha) \quad \rho = \alpha \quad (14)$$

(iii) *Maximal current phase* For $\alpha \geq \frac{1}{2}$ and $\beta \geq \frac{1}{2}$,

$$J = \frac{1}{4} \quad \rho = \frac{1}{2} \quad (15)$$

Consider the high density phase. In this phase the exit rate is low and the bulk density is controlled by the right boundary. One can think of this as queue of traffic formed at a traffic light that doesn't let many cars through at a time.

The low density phase is the opposite scenario where the left boundary controls the density through a low input rate of particles. One can think of this as cars being let onto an empty road only a few at a time.

Finally in the maximal current phase the current of particles is saturated *i.e.* increasing α or β any further does not increase the current or change the bulk density. In this phase the density of particles decays from α its value at the left boundary to $1/2$ its value in the bulk as $x^{-1/2}$ where x is the distance from the left boundary.

This phase diagram of the model has many interesting features. Firstly we have both continuous (from high density or low density to maximal current) and discontinuous (from low density to high density) phase transitions even though it is a one-dimensional system. In the former transitions there are discontinuities in the second derivative of the current. In the latter although the current is continuous across the phase transition its first derivative and the bulk density jump. Along the transition line $\alpha = \beta < 1/2$ one has coexistence between a region of the high density phase adjacent to the right boundary and a region of the low density phase adjacent to the left boundary. These results are very suggestive that the current J can be thought of as some free energy. We shall see later through an exact solution how this can be quantified. Also note that throughout the maximal current phase one has long-range, power-law correlations functions *i.e.* long-range correlations are generic. This contrasts with usual behaviour in equilibrium systems where power-law correlations are seen at non-generic, critical points (an exception is the Kosterlitz-Thouless phase that may emerge at low temperature in two-dimensional equilibrium systems).

2.2 Reacting particle systems and applications

We now have a look at reaction-diffusion systems wherein particles can react with each other to form some by-product or more simply annihilate each other. Well-studied reaction systems are



The first reaction signifies that when two A particles meet they react and annihilate each other, the second that the two reagents coalesce. These systems model molecular reactions and the dynamics of laser induced quasiparticles known as excitons [13]. However the particles in this type of system can also represent composite objects such as aggregating traffic jams or, as we shall see, domain walls in phase-ordering kinetics.

Consider first the $A + A \rightarrow \emptyset$ reaction. Clearly the steady state of such a system

is the uninteresting dead state where all particles (except perhaps one) have been annihilated. The true interest lies in the late time regime wherein the system may enter a *scaling* regime. By this it is meant that the system is statistically invariant under rescaling by a typical length scale that depends on time. In this case the length scale can be taken as the typical distance between particles.

For diffusing A particles, known results are that for $d = 1$ the typical distance between particles grows as $t^{1/2}$ or equivalently the density of a particles decreases as $\rho \sim t^{-1/2}$. We shall recover this result in the next section. The result differs from a naive mean-field description obtained by assuming

$$\frac{\partial \rho}{\partial t} \propto -\rho^2$$

which would predict $\rho \sim t^{-1}$. A similar density decay law holds for the $A + A \rightarrow A$ process and it has been shown that the two processes are basically equivalent [14–17]. In addition to having a range of applications, diffusive reaction systems have served as prototypes for the development of a variety of theoretical tools including field-theoretic techniques [18] and the renormalisation group [19] and exact methods in one dimension [1,7].

One can also consider *ballistic* particle motion. In this class of models, particles move deterministically with constant velocity and on meeting have some probability of coalescing into one particle or annihilating. A seminal paper by Elskens and Frisch [20] that considered the one-dimensional deterministic case where right moving and left moving particles always annihilate on contact, showed the decay depends on the initial densities of the two species. In particular, $\rho \sim t^{-1/2}$ only if there are equal initial densities of the right-moving and left-moving particles. Ballistic models apply to chemical reactions when the inter-reactant distance is less than what would be the mean free path of particles. Such models may also be applied to various domain growth problems [21] and as we shall describe in section 6, the smoothing of a growing interface [22].

3 Theory of Stochastic Processes

Having now given a rough overview of some of the interest in low dimensional nonequilibrium systems, the rest of these lectures will be aimed at a given a deeper understanding of how these phenomena come about in some of the simple models we have discussed. In this section we give a brief introduction to stochastic processes focussing on particular aspects that will be relevant to the models to be studied in detail in later sections.

We consider a system that can be in a finite number of microscopic configurations and whose configuration changes according to transition rates. The simplest example is of a particle performing a random walk in continuous time on a one-dimensional lattice: the particle hops to the right with rate p and to the left with rate q . (The meaning of a ‘rate’ W is that in an infinitesimal time interval dt an event happens with probability Wdt .) Since probability is conserved we can write a continuity equation for the probability which is referred to as ‘the master equation’

$$\frac{\partial P(x, t)}{\partial t} = pP(x - 1, t) + qP(x + 1, t) - (p + q)P(x, t) \quad (17)$$

The first two terms on the right hand side represent ‘rates in’ from other configurations (*i.e.* different positions of the particle); the last term represents the rate out of the given configuration. Note that the master equation is linear in the probabilities.

For the case of the random walker, the master equation (17) can be solved analytically: it is a diffusion equation in discrete space but continuous time. If we consider a periodic lattice of N sites (site $N + 1$ is identified with site 1) the preferred method is to calculate the Fourier modes. Defining

$$\tilde{P}(k, t) = \frac{1}{N} \sum_{x=1}^N z_k^x P(x, t) \quad \text{with} \quad z_k = e^{2\pi i k / N} \quad (18)$$

yields from (17)

$$\frac{d\tilde{P}(k, t)}{dt} = \lambda_k \tilde{P}(k, t) \quad \text{where} \quad \lambda_k = p(z_k - 1) + q(z_k^{-1} - 1). \quad (19)$$

Thus

$$P(x, t) = \sum_{k=1}^N e^{\lambda_k t} z_k^{-x} \tilde{P}(k, 0) \quad \text{with} \quad \tilde{P}(k, 0) = \frac{1}{N} \sum_{x=1}^N z_k^x P(x, 0). \quad (20)$$

The steady state corresponds to the mode $k = N$ ($\lambda = 0$). The eigenvalues λ_k yield decay times $\tau_k = 1 / |\text{Re}\lambda_k|$ of each mode. For k finite and N large

$$\lambda_k \simeq (p - q) \frac{2\pi i k}{N} - (p + q) \frac{4\pi^2 k^2}{N^2} \quad (21)$$

Thus the equilibration time goes like $\tau \sim N^z$ where the dynamic exponent $z = 2$ as expected of a diffusion process.

Exercise 1: Random walker on the 1d lattice

- (a) Review the solution of equation (17) using Fourier modes described above. Show that if the initial condition is $P(x, 0) = \delta_{x, x_0}$ the probability distribution at

time t is given by

$$P(x, t|x_0, 0) = \frac{1}{N} \sum_{k=1}^N \exp \left(\lambda_k t - \frac{2\pi i k(x - x_0)}{N} \right) .$$

where λ_k is given by (19)

If you are unfamiliar with the discrete Fourier transform, you should first show that for $1 \leq k, \ell \leq N$

$$\frac{1}{N} \sum_{x=1}^N z_x^{k-\ell} = \delta_{k,\ell}$$

and hence

$$\tilde{f}(k) = \frac{1}{N} \sum_{x=1}^N z_k^x f(x) \quad \Leftrightarrow \quad f(x) = \sum_{k=1}^N z_x^{-k} \tilde{f}(k)$$

where z_k is as given by equation (18).

(b) Consider now the same random walk problem but on an infinite rather than periodic lattice. Show from equation (17) that the generating function $F(z, t) = \sum_{x=-\infty}^{\infty} P(x, t)(q/p)^{x/2} z^x$ obeys

$$\frac{\partial F(z, t)}{\partial t} = [-(p+q) + \sqrt{pq}(z + z^{-1})] F(z, t)$$

and hence

$$F(z, t) = F(z, 0) \exp[-(p+q)t] \exp[\sqrt{pq}(z + z^{-1})t] . \quad (\text{E1.1})$$

Given that the generating function of modified Bessel functions of the first kind $I_n(x)$ is defined as

$$\sum_{n=-\infty}^{\infty} I_n(x) z^n = \exp \left[\frac{1}{2}(z + z^{-1})x \right] ,$$

show by expanding (E1.1) that the general solution for the random walk problem is

$$P(x, t) = \exp[-(p+q)t] \sum_{\ell=-\infty}^{\infty} \left(\frac{p}{q} \right)^{\frac{x-\ell}{2}} P(\ell, 0) I_{x-\ell}(2\sqrt{pq}t) . \quad (\text{E1.2})$$

Some of the properties of the modified Bessel functions $I_n(x)$ can be gleaned by considering the special case of a symmetric random walker that begins at the origin, *i.e.* the case $p = q = \frac{1}{2}$ and $P(x, 0) = \delta_{x,0}$. Then, $P(x, t) = \exp(-t)I_x(t)$. Show then that the property $I_n(0) = \delta_{n,0}$ immediately follows, as does the fact that

$I_{-n}(t) = I_n(t)$. Also, show from (17) that the Bessel functions satisfy the differential equation

$$\frac{dI_n(x)}{dx} = \frac{1}{2} [I_{n-1}(x) + I_{n+1}(x)] .$$

More generally we consider ‘many-body’ problems. For example a system of many particles on a lattice obeying stochastic dynamical rules. For concreteness we consider the simple example of the one-dimensional Ising model in which at each site i there is a spin $S_i = \pm 1$ and periodic boundary conditions are imposed.

As mentioned in the introduction the dynamics of an equilibrium model is usually chosen to satisfy detailed balance. In the case of the Ising model under spin-flip dynamics, whereby each spin can flip with a certain rate according to the directions of the neighbouring spins, the detailed balance condition on the spin-flip rates of spin S_i at site i reads

$$\frac{W(S_i \rightarrow -S_i)}{W(-S_i \rightarrow S_i)} = \exp [-2\beta(S_{i-1} + S_{i+1})S_i] \quad (22)$$

(We have taken $E = -\sum_i S_i S_{i+1}$). In *Glauber* dynamics (22) is satisfied by choosing

$$W(S_i \rightarrow -S_i) = \frac{1 - S_i \tanh [\beta(S_{i-1} + S_{i+1})]}{2} \quad (23)$$

as is easily verified. Then, in the $T = 0$ limit the spin flips for a down-spin ($S_i = -1$) at site i occur with the rates indicated in Figure 4 and similarly for up-spins at $T = 0$. Note the final transition where the spin flips against both its neighbours is forbidden. Thus domains of aligned spins can not break up. The domain walls between aligned domains *i.e.* neighbouring pairs of spins $\downarrow \uparrow$ or $\uparrow \downarrow$ make random walks on the bonds of the original lattice and annihilate when they meet. As noted above, this process of diffusing ‘particles’ (here the domain walls) that annihilate on meeting is sometimes denoted $A+A \rightarrow \emptyset$. The solution for the mean domain length has been known for some time [23,14]—basically it can be solved by considering the random walk performed by the length of a domain (distance between neighbouring particles).

To see the solution for the mean domain size within the kinetic Ising model [24] consider the master equation which can be written

$$\frac{\partial P(\mathcal{C}, t)}{\partial t} = - \sum_i P(\mathcal{C}, t) W(S_i \rightarrow -S_i) + \sum_i P(\mathcal{C}_i, t) W(-S_i \rightarrow S_i) \quad (24)$$

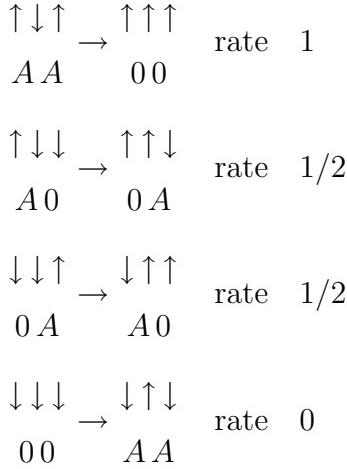


Fig. 4. $T = 0$ dynamics of the Ising model under Glauber dynamics. Also indicated is the interpretation of domain walls as annihilating particles.

where \mathcal{C} is a configuration of the Ising spins and \mathcal{C}_i is the same configuration with spin S_i flipped. The number of domain walls is given by $\sum_i (1 - S_i S_{i+1})/2$ so to study the coarsening process, in which domain walls are eliminated and aligned domains increase in size, one considers the equal time correlation function $C_k(t) = \langle \frac{1}{N} \sum_i S_i(t) S_{i+k}(t) \rangle$ where the average indicates an average over initial conditions and possible histories of the stochastic dynamics. It can be shown that C_k obeys a discrete diffusion equation

$$\frac{\partial C(k, t)}{\partial t} = -2C(k, t) + C(k+1, t) + C(k-1, t) \quad \text{for } k > 0 \quad (25)$$

with boundary condition $C(0, t) = 1$.

The fact that we obtain a closed set of equations for two point correlation functions is a very happy property that allows one to solve easily for these correlation functions—basically (25) is an equation of the same form as (17) but with a boundary condition corresponding to a source of walkers at site 0: see [25,26] for details. Note that the method generalises to finite temperature but not to higher dimensions. Actually higher point correlation functions are more difficult to calculate; nevertheless it has been shown that the one-dimensional Glauber model can be turned into a free fermion problem which then implies, in principle at least, that any correlation function can be calculated [27].

Remarkably, the full domain size probability distribution has been explicitly calculated for the one-dimensional q -state Potts model, which includes the Ising model as the case $q = 2$ [28]. (Note that a calculation such as Exercise 2

only calculates the first moment of the domain sizes). The dynamics of domain walls in the q -state Potts model, represented as A particles, corresponds to diffusion and, on meeting, reaction according to

$$A + A \rightarrow \begin{cases} A & \text{with probability } (q-2)/(q-1) \\ \emptyset & \text{with probability } 1/(q-1) \end{cases} \quad (26)$$

To understand this equation note that when a domain is eliminated each of the neighbouring domains may be in one of $q-1$ states so that they have probability $1/(q-1)$ of being in the same state and therefore coalescing. Thus for $q=2$ we recover $A + A \rightarrow \emptyset$ and for $q \rightarrow \infty$ (infinite state Potts model) we recover $A + A \rightarrow A$.

Exercise 2: Time dependence of the 1d Ising model

- (a) The mean magnetisation $M(t)$ in the 1d Ising model is defined as

$$M(t) = \frac{1}{N} \sum_{j=1}^N \langle S_j \rangle \equiv \frac{1}{N} \sum_{\{\mathcal{C}\}} P(\mathcal{C}, t) \sum_{j=1}^N S_j(\mathcal{C})$$

where N is the number of spins on the lattice, $\{\mathcal{C}\}$ is the set of all 2^N possible spin combinations and $S_i(\mathcal{C})$ is the value of the spin at site i , in configuration \mathcal{C} . Show for general single spin-flip dynamics as described by (24) that the magnetisation obeys the differential equation

$$\frac{dM}{dt} = -\frac{2}{N} \sum_{\{\mathcal{C}\}} P(\mathcal{C}, t) \sum_{i=1}^N S_i W(S_i \rightarrow -S_i).$$

Under Glauber dynamics defined by equation (23) show that

$$\frac{dM}{dt} = -(1 - \tanh 2\beta) M(t)$$

and hence that $M(t) = M(0) \exp(-[1 - \tanh 2\beta]t)$. Also comment on the finite- and zero-temperature behaviour (recalling that β is inverse temperature).

Hint: you will need to argue that the relation $\sum_i \tanh \beta(S_{i-1} + S_{i+1}) = \sum_i S_i \tanh 2\beta$ holds for any (periodic) combination of spins.

- (b) Show that the mean density of domain walls $n_D(t)$ in the 1d Ising model can be expressed using the spin correlation function $C(k, t)$ as $n_D(t) = \frac{1}{2}[1 - C(1, t)]$. Under zero-temperature Glauber dynamics, the evolution of $C(k, t)$ is described by the set of difference equations (25) which has the stationary solution $C(k) = 1 \forall k \geq 0$. Verify this solution, and explain its physical meaning.

To obtain the time-dependence of $C(k, t)$ we introduce a function $\epsilon(k, t)$ through $C(k, t) = 1 - \epsilon(k, t)$. The time-evolution is governed by equation (17) with $P(k, t) = \epsilon(k, t)$, $p = q = 1$ and subject to the boundary condition $\epsilon(0, t) = 0 \forall t$.

This boundary condition can be satisfied through an appropriate choice of the initial conditions $\epsilon(k, 0)$ in the ‘unphysical’ region $k < 0$ (this is equivalent to using the Method of Images [29]). Using the general solution (E1.2) and the properties of the modified Bessel functions derived in exercise 1, show that $\epsilon(0, t) = 0 \forall t$ if $\epsilon(-k, 0) = \epsilon(k, 0)$. Hence show that

$$C(k, t) = 1 - \exp(-2t) \sum_{\ell=1}^{\infty} [I_{k-\ell}(2t) - I_{k+\ell}(2t)]$$

is the solution for the spin correlation function that has $C(0, t) = 1 \forall t$ and with the initial spin orientations uncorrelated, *i.e.* $C(k, 0) = \delta_{k,0}$. Show that this implies that for these initial conditions, $n_D(t) = \frac{1}{2} \exp(-2t)[I_0(2t) + I_1(2t)]$.

Finally, using the asymptotic form of the modified Bessel functions

$$I_n(x) = \frac{\exp(x)}{\sqrt{2\pi x}} \left[1 + \sum_{k=1}^{\infty} \frac{(-1)^k}{k!(8x)^k} \prod_{j=1}^k (4n^2 - (2j-1)^2) \right]$$

show that the long-time behaviour of $n_D(t)$ is $n_D(t) \sim (4\pi t)^{-1/2} + O(t^{-3/2})$.

In order to formalise stochastic processes in general we consider a master equation

$$\frac{dP(\mathcal{C}, t)}{dt} = \sum_{\mathcal{C}' (\neq \mathcal{C})} P(\mathcal{C}') W(\mathcal{C}' \rightarrow \mathcal{C}) - \sum_{\mathcal{C}' (\neq \mathcal{C})} P(\mathcal{C}) W(\mathcal{C} \rightarrow \mathcal{C}') \quad (27)$$

where $W(\mathcal{C} \rightarrow \mathcal{C}')$ is the rate of transition from configuration \mathcal{C} to \mathcal{C}' . It is useful to combine the transition rates into a single matrix

$$M(\mathcal{C}, \mathcal{C}') = W(\mathcal{C}' \rightarrow \mathcal{C}) \quad \text{for } \mathcal{C}' \neq \mathcal{C} \quad (28)$$

$$M(\mathcal{C}, \mathcal{C}) = - \sum_{\mathcal{C}'} W(\mathcal{C} \rightarrow \mathcal{C}') \quad (29)$$

so that we can write

$$\frac{dP(\mathcal{C}, t)}{dt} = \sum_{\mathcal{C}'} M(\mathcal{C}, \mathcal{C}') P(\mathcal{C}', t). \quad (30)$$

Now let us introduce a ‘bra-ket’ notation. Let the vector of probabilities at time t (one component for each configuration) be $|P\rangle_t$. Thus the probability

of the system being in configuration \mathcal{C} at time t is $\langle \mathcal{C}|P\rangle_t$ and we can write the master equation as

$$\frac{d|P\rangle_t}{dt} = M|P\rangle_t . \quad (31)$$

Thus the master equation looks something like a Schrödinger equation with ‘imaginary time’ and H replaced by $-M$ (this is why M is sometimes referred to as a Hamiltonian). However it should be recalled that in quantum mechanics it is the modulus squared of the components $|P\rangle_t$ that are probabilities whereas here the components of $|P\rangle_t$ are probabilities. See [30,7,31], for example, for more details.

The formal solution of the master equation (31) is

$$|P\rangle_t = \exp(Mt)|P\rangle_0 \quad (32)$$

where $|P\rangle_0$ gives the initial conditions. However, a more useful way of dealing with the problem is to consider the eigenvectors of the transition matrix M . The first thing to note is that since M is not Hermitian, in general, it has different left and right eigenvectors

$$M|\phi_\lambda\rangle = \lambda|\phi_\lambda\rangle \quad (33)$$

$$\langle\psi_\lambda|M = \lambda\langle\psi_\lambda| . \quad (34)$$

These satisfy ‘bi-orthogonality’

$$\langle\psi_\lambda|\phi_\mu\rangle = \delta_{\lambda,\mu} , \quad (35)$$

and in principle (assuming M can be diagonalised) we may write

$$1\!\!1 = \sum_\lambda |\phi_\lambda\rangle\langle\psi_\lambda| \quad (36)$$

$$M = \sum_\lambda \lambda|\phi_\lambda\rangle\langle\psi_\lambda| . \quad (37)$$

Then we have using (32), (36) and (33)

$$|P\rangle_t = \sum_{n=0}^{\infty} \frac{M^n t^n}{n!} |P\rangle_0 = \sum_\lambda \exp(\lambda t) |\phi_\lambda\rangle\langle\psi_\lambda| |P\rangle_0 . \quad (38)$$

Note that the real parts of all eigenvalues λ are negative except for one eigenvalue which is zero. The reason for this is often referred to as the Perron-Frobenius theorem [32]. This theorem holds for a matrix with non-negative entries where a sufficiently large power of the matrix has all positive entries. It

states that the maximum eigenvalue is non-degenerate and the corresponding left and right eigenvectors have positive entries.

In our context one can relate the spectrum of M to that of non-negative matrix \tilde{M} obtained by adding some suitable multiple (say minus the diagonal element with the largest magnitude) of the identity matrix to M . The assumption that a sufficiently large power of \tilde{M} has all positive entries is equivalent to the assumption that the (finite) system is ergodic *i.e.* any configuration can be reached from any other after sufficient time. In that case the system will have a unique steady state so that the zero eigenvalue cannot be degenerate and the steady state eigenvector has positive elements which correspond to probabilities.

In principle, all probabilities at all times can be found if one can diagonalise the matrix M . Unfortunately this is only possible in a few isolated cases. Generally this corresponds to many-particle systems where the particles do not interact or certain ‘integrable’ systems that can be solved via the Bethe ansatz.

The Bethe ansatz was originally used in the context of a spin-chain model for magnetism [33] and is suitable for a one-dimensional lattice system in which the number of particles is conserved. It is basically a generalisation of the Fourier transform. Let us briefly discuss it for the case of the ASEP. The idea is to guess the following form for eigenvectors ϕ

$$\phi(x_1, x_2, \dots, x_M) = \sum_Q A(Q) z_1^{x_{Q(1)}} z_2^{x_{Q(2)}} \cdots z_M^{x_{Q(M)}} \quad (39)$$

in which x_i is the position of particle i on a lattice, and $1 \leq x_1 < x_2 < x_3 \dots < x_M \leq N$ with N the lattice size once again. The sum is over all permutations Q of $(1, 2, \dots, M)$ and $A(Q)$ is some amplitude. One uses the master equation to determine relations that must be satisfied by $\phi(x_1, \dots, x_M)$ in its unphysical regions, *e.g.* where two particles occupy the same site and $x_i = x_{i+1}$ for some i . After some manipulation, one arrives at a set of nonlinear equations that must be simultaneously satisfied by all the ‘momenta’ z_i . An early account of this method in the context of stochastic processes is given in [34]. The technique is also described in [7,35]. However even for the so-called ‘integrable’ systems where the Bethe ansatz works it is actually very difficult to extract the explicit eigenvectors.

Of course, it may not be possible to solve a model exactly, and in this situation one often turns to approximation schemes. For example, one can try a ‘short time’ expansion—we simply truncate the power series defining the exponential

of M in (32) after m terms

$$|P\rangle_t \simeq \sum_{n=0}^m \frac{M^n t^n}{n!} |P\rangle_0 . \quad (40)$$

The finite number of terms m on the right hand side can be calculated. From the series one can try to estimate, for example, the dynamical exponent [36].

A project less ambitious than solving the full dynamics is to calculate the steady state probabilities (the eigenvector with eigenvalue 0). We denote the steady state by dropping the subscript t so that $|P\rangle$ is the eigenvector with eigenvalue zero

$$\frac{d|P\rangle}{dt} = M|P\rangle = 0 , \quad (41)$$

and its components $P(\mathcal{C})$ are the steady state probabilities. Thus one has the balance conditions

$$\sum_{\mathcal{C}'} W(\mathcal{C} \rightarrow \mathcal{C}') P(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}' \rightarrow \mathcal{C}) P(\mathcal{C}') . \quad (42)$$

Let us review some simple ways to satisfy (42). First of all one has the case of detailed balance where

$$W(\mathcal{C} \rightarrow \mathcal{C}') P(\mathcal{C}) = W(\mathcal{C}' \rightarrow \mathcal{C}) P(\mathcal{C}') . \quad (43)$$

However to check this condition *i.e.* to check whether detailed balance is satisfied we first need to know the steady state! However there is an equivalent set of conditions called ‘Kolmogorov criteria’ which state that detailed balance is obeyed if and only if the transition rates satisfy

$$\begin{aligned} & W(\mathcal{C}_1 \rightarrow \mathcal{C}_2) W(\mathcal{C}_2 \rightarrow \mathcal{C}_3) \dots W(\mathcal{C}_n \rightarrow \mathcal{C}_1) \\ & = W(\mathcal{C}_1 \rightarrow \mathcal{C}_n) W(\mathcal{C}_n \rightarrow \mathcal{C}_{n-1}) \dots W(\mathcal{C}_2 \rightarrow \mathcal{C}_1) \end{aligned} \quad (44)$$

for *every* possible cycle in configuration space $\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_n, \mathcal{C}_1$.

That (43) implies (44) is very simple to show. To show that the converse is also true is most simply achieved [37,38] by using (43) to determine $P(\mathcal{C})$. Then, one finds that $P(\mathcal{C})$ is unique if and only if (44) is satisfied.

Let us consider some of the implications of the detailed balance condition. First note that when one has detailed balance then in the steady state there is no net flow of probability between any two configurations. Since there is no flow of probability there is nothing to distinguish the forwards direction in time from backwards direction. Therefore running the systems backwards in

time will not change, for example, any two time correlation functions. Thus the system is said to be *reversible*.

Now consider the simple problem of a single random walker on a periodic one-dimensional lattice, studied at the beginning of this section. The steady state is given by equal probability of the walker occupying each site. However, one does not have detailed balance as defined above unless the hop rates are symmetric $p = q$. But one knows that the only effect of $p \neq q$ is to impose a drift. Clearly with a drift the system is not reversible. But the system is reversible under simultaneous reversal of time and parity (*i.e.* direction): the parity operation results in defining the image of position x as $x^* = N + 1 - x$. Then trivially

$$W(x \rightarrow x+1)P(x) = W(N-x \rightarrow N-x+1)P(N-x) \quad (45)$$

since in the steady state $P(x)$ is constant in space and both transition rates are equal to p .

More generally an *extended* detailed balance condition can pertain as defined in [39]:

$$W(\mathcal{C} \rightarrow \mathcal{C}')P(\mathcal{C}) = W(\mathcal{C}'^* \rightarrow \mathcal{C}^*)P(\mathcal{C}'^*) \quad (46)$$

where \mathcal{C}^* is the image configuration of \mathcal{C} under a reversible mapping. One requires $(\mathcal{C}^*)^* = \mathcal{C}$ and

$$\sum_{\mathcal{C}'} W(\mathcal{C} \rightarrow \mathcal{C}') = \sum_{\mathcal{C}'} W(\mathcal{C}^* \rightarrow \mathcal{C}') . \quad (47)$$

Again one can construct an equivalent condition as follows [40]

$$\begin{aligned} & W(\mathcal{C}_1 \rightarrow \mathcal{C}_2)W(\mathcal{C}_2 \rightarrow \mathcal{C}_3) \dots W(\mathcal{C}_n \rightarrow \mathcal{C}_1) \\ &= W(\mathcal{C}_1^* \rightarrow \mathcal{C}_n^*)W(\mathcal{C}_n^* \rightarrow \mathcal{C}_{n-1}^*) \dots W(\mathcal{C}_2^* \rightarrow \mathcal{C}_1^*) \end{aligned} \quad (48)$$

for *every* possible cycle in configuration space $\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3, \dots, \mathcal{C}_n$ along with the additional condition (47).

The condition (46) is known in the probabilistic literature as *dynamic reversibility* [38]. More recently it has appeared in the physics literature under the name *pairwise balance* [41]. It holds for example in the ASEP on a ring where the image configuration is obtained by the parity operation.

3.1 Formal solution for the steady state

In this subsection our aim is to derive the general solution for the steady state (41) for an arbitrary transition rate matrix M . Although the solution is too general to be of any practical use it is instructive to see how a quantity analogous to a partition function naturally arises.

As it stands, the set of linear equations (41) is underdetermined because the determinant of M is zero (one of its eigenvalues is zero). However, we know that a probability distribution must be properly normalised, so consider instead the equation

$$\widetilde{M}^{(i)}|P\rangle = |i\rangle \quad (49)$$

in which $\widetilde{M}^{(i)}$ is the matrix obtained from $-M$ (the minus sign is introduced for convenience below) by replacing the i^{th} row with all ones, *i.e.* the vector $(1, 1, 1, \dots, 1)$. The ket vector $|i\rangle$ is the basis vector corresponding to configuration i . This set of equations can now be solved and we do so using Cramer's rule. This states that the probability of the system being in configuration \mathcal{C}_j in the steady state is

$$P(\mathcal{C}_j) = \frac{\det \widetilde{M}^{(i;j)}}{\det \widetilde{M}^{(i)}} \quad (50)$$

in which the matrix $\widetilde{M}^{(i;j)}$ is obtained from $\widetilde{M}^{(i)}$ by replacing column j with a vector with a 1 at position j and zeros everywhere else. For simplicity we choose $i = j$, and to be clear we write out $\widetilde{M}^{(j;j)}$ explicitly.

$$\widetilde{M}^{(j;j)} = \begin{bmatrix} -M_{1,1} & \cdots & -M_{1,j-1} & 0 & -M_{1,j+1} & \cdots & -M_{1,n} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -M_{j-1,1} & \cdots & -M_{j-1,j-1} & 0 & -M_{j-1,j+1} & \cdots & -M_{j-1,n} \\ 1 & \cdots & 1 & 1 & 1 & \cdots & 1 \\ -M_{j+1,1} & \cdots & -M_{j+1,j-1} & 0 & -M_{j+1,j+1} & \cdots & -M_{j+1,n} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -M_{n,1} & \cdots & -M_{n,j-1} & 0 & -M_{n,j+1} & \cdots & -M_{n,n} \end{bmatrix}. \quad (51)$$

We note that the determinant $\det \widetilde{M}^{(j;j)}$ is equal to the determinant of the matrix obtained from $\widetilde{M} = -M$ by removing row j and column j . This determinant is called a cofactor of \widetilde{M} and will be written $f_j \equiv f(\mathcal{C}_j)$. Furthermore, we observe that the determinant in the denominator of (50) is the sum of all

these cofactors. That is

$$Z = \sum_{j=1}^n f_j \quad (52)$$

so that

$$P(\mathcal{C}_j) = \frac{f_j}{Z}. \quad (53)$$

We thus identify the cofactor f_j with the *steady-state weight* of configuration \mathcal{C}_j and Z as a *normalisation* for the stochastic process. In an equilibrium system, Z is related to the partition function $Z_{eq} = \sum_{\mathcal{C}} \exp(-\beta E(\mathcal{C}))$. However, the normalisation Z obtained using the above procedure is not guaranteed to be identical to Z_{eq} due to the possibility of common factors present in all the weights f_j and hence Z . With this understood, (52) extends the notion of a partition function to nonequilibrium systems.

3.2 Relationship of the steady-state normalisation to eigenvalues of the transition-rate matrix

We now note an interesting and, as far as we are aware, little-known result that relates the normalisation Z (52) to the eigenvalues of the transition matrix. The relation reads

$$Z = \prod_{\lambda_j \neq 0} (-\lambda_j) \quad (54)$$

in which the product is over the eigenvalues of the transition rate M except the zero eigenvalue.

This result is obtained by expanding the characteristic polynomial $\det(\lambda \mathbb{1} - M)$ in powers of λ . One finds [42]

$$\det(\lambda \mathbb{1} - M) = (-)^n \left(\det M + (-)^n \lambda \sum_{j=1}^n f_j + O(\lambda^2) \right) \quad (55)$$

with f_j as defined above. Given that $\det M = 0$ and $Z = \sum_j f_j$ we find that

$$Z = \lim_{\lambda \rightarrow 0} \frac{\det(\lambda \mathbb{1} - M)}{\lambda} = \lim_{\lambda \rightarrow 0} \frac{\prod_j (\lambda - \lambda_j)}{\lambda} = \prod_{\lambda_j \neq 0} (-\lambda_j) \quad (56)$$

where the last step follows because one, and only one, eigenvalue of M is zero (at least if the process is ergodic).

3.3 Nonequilibrium phase transitions

We now consider the existence of *phase transitions* in a stochastic process. As in equilibrium systems, we identify phase transitions through discontinuities in macroscopic quantities or their derivatives. Furthermore, at a first-order (discontinuous) transition we expect phase coexistence and at a continuous transition divergences in length and time scales.

In terms of eigenvalues of the transition matrix M , a phase transition would be indicated by the clustering of one or more eigenvalues towards zero. For example as a discontinuous transition is approached one would expect long-lived ‘excited’ states since the decay time of an eigenstate of M is inversely proportional to the real part of the corresponding eigenvalue. These long-lived states can be thought of as metastable states and the approach of an eigenvalue to zero in the thermodynamic (infinite system-size) limit suggests phase coexistence. Near a continuous transition one has diverging time scales (as manifested by *e.g.* a power-law decay of an autocorrelation function) so one expects a continuous spectrum of eigenvalues whose real parts are close to zero.

Bearing this in mind, we note that equation (54) implies that the steady-state normalisation Z also approaches zero at a phase transition in the thermodynamic limit. Such a scenario is analogous to Yang-Lee theory of equilibrium phase transitions, in which it has been rigorously shown that zeros of the grand canonical partition function in the complex-fugacity plane converge towards a point on the positive real axis that indicates the value of the fugacity at which a phase transition occurs. Similar properties are also displayed by the zeros of the canonical partition function in the complex-temperature plane (these are also known as Fisher zeros). Hence, it would seem likely from (54) and the above considerations that zeros of a steady-state nonequilibrium normalisation in the complex plane of some control parameter would also converge to the real axis at a nonequilibrium phase transition. This would also imply nonanalyticities in a macroscopic variable averaged with respect to the steady-state probability distribution function.

This idea has been pursued in the context of an asymmetric exclusion process [43]. In this case, the steady-state normalisation was solved for its zeros in the complex-fugacity plane and indeed they were found to approach the real axis for values of the model parameters that corresponded to a phase transition. Additionally, a similar approach has been tried in the context of directed percolation [44], a further lattice model that exhibits a nonequilibrium phase transition (see *e.g.* [31] for a review).

This concludes our overview of stochastic processes. We will shortly move on

to the specific models we are going to study. As mentioned in the introduction the ‘ q -deformed Harmonic Oscillator’ plays a central role in the solution of both these models.

4 Intermezzo: What is a q -deformed Harmonic Oscillator?

First let us recall the quantum harmonic oscillator well known from undergraduate physics. The Hamiltonian is

$$\hat{H} = \frac{1}{2}\hat{x}^2 + \frac{1}{2}\hat{p}^2 \quad (57)$$

where we have lazily set all constants m, \hbar, π etc to unity and where $\hat{\cdot}$ denotes an operator. One way to treat the problem is to introduce two new operators \hat{a}, \hat{a}^\dagger through

$$\hat{x} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger) \quad \hat{p} = -\frac{i}{\sqrt{2}}(\hat{a} - \hat{a}^\dagger). \quad (58)$$

Then inserting these definitions into the commutation relation $[\hat{x}, \hat{p}] = i\mathbb{1}$ yields

$$\hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \mathbb{1}. \quad (59)$$

Also the Hamiltonian (57) becomes

$$\hat{H} = \hat{a}^\dagger\hat{a} + \frac{1}{2}. \quad (60)$$

The operators \hat{a}, \hat{a}^\dagger are, of course, raising and lowering operators. More generally they are bosonic operators, the defining property of which is the commutation relation (59). In the number (or energy) basis they obey

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad \text{for } n \geq 0. \quad (61)$$

Thus in this basis $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$ and the Hamiltonian is diagonal. The number n labels the energy eigenstates. The quantised energy excitations obey Bose statistics and the operators (61) create and annihilate bosons respectively.

The Hermite polynomials come into play when we consider the projection of an energy eigenstate onto the position eigenbasis defined by

$$\hat{x}|x\rangle = x|x\rangle. \quad (62)$$

Then

$$\langle x|n\rangle = e^{-x^2} H_n(x) \quad (63)$$

where $H_n(x)$ is the Hermite polynomial of degree n .

We now consider a ‘deformation’ of (59) by introducing a parameter q [45]

$$\hat{a}\hat{a}^\dagger - q\hat{a}^\dagger\hat{a} = \mathbb{1} . \quad (64)$$

Observe that taking $q = 1$ recovers bosonic operators whereas $q = -1$ gives fermionic operators. Thus it was originally hoped that the q -deformed operators might describe some new excitations interpolating between fermions and bosons.

The operators \hat{a} and \hat{a}^\dagger now operate on basis vectors $|n\rangle$ (with $n = 0, 1, 2, \dots$) as follows:

$$\hat{a}^\dagger|n\rangle = \sqrt{\frac{1-q^{n+1}}{1-q}}|n+1\rangle \quad (65)$$

$$\hat{a}|n\rangle = \sqrt{\frac{1-q^n}{1-q}}|n-1\rangle . \quad (66)$$

Thus $\hat{a}^\dagger\hat{a}$, which is the analogue of the energy operator, is diagonal in this basis

$$\hat{a}^\dagger\hat{a}|n\rangle = \frac{1-q^n}{1-q}|n\rangle . \quad (67)$$

The eigenstates of the ‘position operator’ $\hat{x} = \hat{a} + \hat{a}^\dagger$ are given by

$$\hat{x}|x\rangle = \frac{2x}{\sqrt{1-q}}|x\rangle . \quad (68)$$

Finally, we identify the q -Hermite polynomials as

$$H_n(x|q) = \langle x|n\rangle . \quad (69)$$

4.1 Properties of q -Hermite polynomials

Using (65,66) and (69) it is straightforward to derive a recurrence relation

$$\sqrt{1-q^{n+1}}H_{n+1}(x|q) - 2xH_n(x|q) + \sqrt{1-q^n}H_{n-1}(x|q) = 0 . \quad (70)$$

This can be compared to the usual recurrence relation for Hermite polynomials

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0 . \quad (71)$$

To make the connection between q -Hermite and ordinary Hermite polynomials we would like the recurrence relations to coincide in the limit $q \rightarrow 1$. The prescription is

$$H_n(x|q) \rightarrow \frac{((1-q)/2)^{n/2}}{(q; q)_n^{1/2}} H_n(\sqrt{(1-q)/2} x) \quad (72)$$

in which both the Hermite polynomial $H_n(x|q)$ and the independent variable x are transformed. The factors of $\sqrt{2}$ that appear can be traced back to the fact that we set $\hat{x} = (\hat{a} + \hat{a}^\dagger)/\sqrt{2}$ when doing the quantum mechanics, but we take $\hat{x} = \hat{a} + \hat{a}^\dagger$ in the q -deformed case.

Explicit formulæ for $\langle x|n \rangle$ can be found using a generating function technique, the details of which differ slightly depending on whether $q < 1$ or $q > 1$. Here we discuss in detail the case $q < 1$.

First we define a generating function $\tilde{G}(x, \lambda)$ for the q -Hermite polynomials

$$\tilde{G}(x, \lambda) = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{(q; q)_n}} \langle x|n \rangle . \quad (73)$$

where have introduced a ‘ q -factorial’ notation defined through

$$(a; q)_n = \prod_{j=0}^{n-1} (1 - aq^j) \quad (74)$$

$$(a; q)_0 = 1 . \quad (75)$$

We later encounter products of these factorials for which we use a standard shorthand [46]:

$$(a, b, c, \dots ; q)_n = (a; q)_n (b; q)_n (c; q)_n \dots . \quad (76)$$

The q -factorial in (73) is introduced for convenience as will now become apparent.

We obtain a functional relation for $\tilde{G}(x, \lambda)$ by multiplying both sides of equation (70) by $\lambda^n/\sqrt{(q; q)_n}$ and performing the required summations:

$$\tilde{G}(x, q\lambda) = (\lambda^2 - 2\lambda x + 1) \tilde{G}(x, \lambda) . \quad (77)$$

It is convenient to parameterise the ‘position’ eigenstates by an angle θ where $x = \cos \theta$ and $0 \leq \theta \leq 2\pi$, and to replace $\tilde{G}(x, \lambda)$ by $G(\theta, \lambda)$ (a function of θ). Then (77) becomes

$$G(\theta, \lambda) = \frac{G(\theta, q\lambda)}{(1 - \lambda e^{i\theta})(1 - \lambda e^{-i\theta})} \quad (78)$$

Since $q < 1$ we can iterate to obtain

$$G(\theta, \lambda) = \frac{1}{(\lambda e^{i\theta}, \lambda e^{-i\theta}; q)_\infty} \quad (79)$$

where we have used the q -factorial notation (76). Note that $G(\theta, 0)$ is just $\langle \theta | 0 \rangle$ which we are free to set to 1.

The infinite product $1/(x; q)_\infty$ has a well-known and easy to verify series representation [46] valid for $|x| < 1$, $q < 1$

$$\frac{1}{(x; q)_\infty} = \sum_{n=0}^{\infty} \frac{x^n}{(q; q)_n} \quad (80)$$

from which, with a little effort, we may extract the form of $\langle \theta | n \rangle$. Expanding both sides of (79) in λ and comparing coefficients we find

$$\langle \theta | n \rangle = \frac{1}{\sqrt{(q; q)_n}} \sum_{k=0}^n \begin{bmatrix} n \\ k \end{bmatrix}_q e^{i(n-2k)\theta} \quad (81)$$

where $\begin{bmatrix} n \\ k \end{bmatrix}_q$ is the q -deformed binomial defined as

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \frac{(q; q)_n}{(q; q)_{n-k}(q; q)_k} \quad (82)$$

when $0 \leq k \leq n$ and zero otherwise. In the limit $q \rightarrow 1$ the q -binomial coefficient is equal to the conventional version $\binom{n}{k}$ familiar from combinatorics.

Important properties of the q -Hermite polynomials are their orthogonality and completeness. It can be shown [46] that the set of q -Hermite polynomials are orthogonal with respect to a weight function $\nu(\theta)$. That is

$$\int_0^\pi d\theta \langle n | \theta \rangle \nu(\theta) \langle \theta | m \rangle = \delta_{n,m} \quad (83)$$

where the weight function is given by

$$\nu(\theta) = \frac{(q, e^{2i\theta}, e^{-2i\theta}; q)_\infty}{2\pi}. \quad (84)$$

Completeness implies we can form a representation of the identity matrix:

$$\int_0^\pi d\theta |\theta\rangle \nu(\theta) \langle \theta | = \mathbb{1}. \quad (85)$$

It is less well known that, in a similar manner to the above exposition, one can obtain explicit forms for q -Hermite polynomials when $q > 1$ [47]. It turns out

that they can be obtained from (81) by making the substitution $\theta \rightarrow \pi/2 - iu$ *i.e.* one replaces $\cos \theta$ by $i \sinh u$ and the parameter u runs from $-\infty$ to ∞ . The weight function that orthogonalises these polynomials is now

$$\nu(u) = \frac{1}{\ln q} \frac{1}{(q^{-1}, -q^{-1}e^{2u}, -q^{-1}e^{-2u}; q^{-1})_\infty}. \quad (86)$$

Exercise 3: Coherent states, the exponential function and their q -deformations

For the ‘traditional’ quantum mechanical raising and lowering operators that satisfy the commutation relation (59) construct the vector $|\mu\rangle = \exp(\mu\hat{a}^\dagger)|0\rangle$. Show that this is a *coherent state*, *i.e.* an eigenvector of the lowering operator \hat{a} with eigenvalue μ .

Now consider a q -coherent state $|\mu\rangle$ satisfying the eigenvalue equation $(1-q)^{1/2}\hat{a}|\mu\rangle = \mu|\mu\rangle$ with \hat{a} and \hat{a}^\dagger the q -deformed raising and lowering operators that obey (64). By solving this eigenvalue equation, show that the q -coherent state $|\mu\rangle$ may be expressed as

$$|\mu\rangle = \exp_q([1-q]^{1/2}\mu\hat{a}^\dagger)|0\rangle$$

where the q -deformation of the exponential function is defined through

$$\exp_q(x) = \sum_{n=0}^{\infty} \frac{x^n}{(q; q)_n}.$$

Show that this series converges always for $q > 1$, for $|x| < 1$ when $q < 1$ and that $\lim_{q \rightarrow 1} \exp_q([1-q]x) = \exp(x)$.

Verify also that when $|q| < 1$ and $\exp_q(x)$ converges, it can also be written as

$$\exp_q(x) = \frac{1}{(x; q)_\infty}.$$

Hint: this is most easily achieved by checking that both the series and product representations of $\exp_q(x)$ satisfy the functional relation $\exp_q(qx) = (1-x)\exp_q(x)$ and that they are numerically equal for a special value of $x = 0$.

Finally, show that

$$\langle \theta | \mu \rangle = \sum_{n=0}^{\infty} \langle \theta | n \rangle \langle n | \mu \rangle = G(\theta, \mu)$$

where $G(\theta, \mu)$ is the generating function of q -Hermite polynomials (73,79).

5 Steady State Solution of Partially Asymmetric Exclusion Process

We now consider in more detail the partially asymmetric exclusion process (PASEP) introduced in Section 2.1. Recall that we discussed some of the properties of the special case where the reverse hop rate q was set to zero and in particular we presented a phase diagram for the model (Figure 3). We now describe how one obtains such a phase diagram exactly for general q . We do this by relating the steady-state probability distribution of the model to products of matrices which can be mapped onto the q -deformed harmonic oscillator ladder operators.

5.1 The matrix product formulation and its quadratic algebra

In this section we review the matrix approach to finding the steady state of the model. The approach has been the subject of lectures at a previous summer school in this series [35] and the reader is referred there for further details. Here the bare essentials of the method are outlined.

Consider first a configuration of particles \mathcal{C} and its steady-state probability $P(\mathcal{C})$. We use as an ansatz for $P(\mathcal{C})$ an ordered product of matrices $X_1 X_2 \dots X_N$ where $X_i = D$ if site i is occupied and $X_i = E$ if it is empty. To obtain a probability (a scalar value) from this matrix product, we employ two vectors $\langle W |$ and $| V \rangle$ in the following way:

$$P(\mathcal{C}) = \frac{\langle W | X_1 X_2 \dots X_N | V \rangle}{Z_N} . \quad (87)$$

Note that here the matrices, bra and ket vectors are in an auxiliary space and are not related to the space of configurations and the probability ket vector we considered earlier. The factor Z_N is included to ensure that $P(\mathcal{C})$ is properly normalised. This latter quantity, analogous to a partition function as was discussed in Section 3, has the following simple matrix expression through which a new matrix $C = D+E$ is defined:

$$Z_N = \langle W | (D + E)^N | V \rangle = \langle W | C^N | V \rangle . \quad (88)$$

Note that if D and E do not commute $P(\mathcal{C})$ is a function of both the number and position of particles on the lattice, as expected for a non-trivial steady state. The algebraic properties of the matrices can be deduced from the master equation for the process [10]. It can be shown that sufficient conditions for equation (87) to hold are

$$DE - qED = D + E \quad (89)$$

$$\alpha\langle W|E = \langle W| \quad (90)$$

$$\beta D|V\rangle = |V\rangle . \quad (91)$$

In this formulation steady state correlation functions are easily expressed. For example, the mean occupation number (density) of site i may be written as

$$\langle \tau_i \rangle = \frac{\langle W|C^{i-1}DC^{N-i}|V\rangle}{Z_N} . \quad (92)$$

To get a feel for why the conditions (89–91) give the correct steady state consider the current J of particles between sites i and $i+1$.

$$J \equiv \langle \tau_i(1 - \tau_{i+1}) \rangle - q\langle (1 - \tau_i)\tau_{i+1} \rangle \quad (93)$$

In the matrix product formulation the current becomes

$$J = \frac{\langle W|C^{i-1}(DE - qED)C^{N-i-1}|V\rangle}{Z_N} . \quad (94)$$

Now using (89) and the fact that $C = D + E$ we find

$$J = \frac{\langle W|C^{N-1}|V\rangle}{Z_N} = \frac{Z_{N-1}}{Z_N} . \quad (95)$$

We see that, as is required in the steady state, the current is independent of the bond chosen.

To see that the current into site one reduces to the same expression we use (90)

$$J = \alpha\langle 1 - \tau_1 \rangle = \frac{\alpha\langle W|EC^{N-1}|V\rangle}{Z_N} = \frac{Z_{N-1}}{Z_N} \quad (96)$$

Also the current out of site N reduces to the same expression using (91)

$$J = \beta\langle \tau_N \rangle = \frac{\beta\langle W|C^{N-1}D|V\rangle}{Z_N} = \frac{Z_{N-1}}{Z_N} \quad (97)$$

Note that the fact that all the above expressions for the current are equivalent is a necessary condition for the matrix formulation to be correct. A sufficient condition is to check that the master equation (41) is satisfied for all 2^N configurations. The algebra (89–91) allows one to do this systematically [10,48].

Our task now is to evaluate the matrix products in the above expressions for Z_N , J and τ_i by applying the rules (89–91).

In [10] the case $q = 0$ was treated by using (89) repeatedly to ‘normal-order’ matrix products: that is, to obtain an equivalent sum of products in which all E matrices appear to the left of any D matrices. For example, consider powers of C

$$\begin{aligned} C^0 &= 1 \\ C^1 &= D + E \\ C^2 &= D^2 + E^2 + (1+q)ED + D + E \\ &\vdots \\ C^N &= \sum_{n=0}^N \sum_{m=0}^{N-n} a_{N,n,m} E^n D^m \end{aligned}$$

Then finding a scalar value would be straightforward using (90) and (91):

$$Z_N = \langle W | C^N | V \rangle = \sum_{n,m} a_{N,n,m} \alpha^{-n} \beta^{-m}. \quad (98)$$

The difficulty with this approach lies in the combinatorial problem of finding the coefficients $a_{N,n,m}$. This was solved for $q = 0$ in [10]. However, the solution (and the problem of actually calculating the current and correlation functions) for arbitrary q remained open for some time although the phase diagram was conjectured [49]. Recently the problem has been overcome by making the connection with the q -Hermite polynomials discussed in Section 4 [50,51].

5.2 Connection with the q -deformed harmonic oscillator

To make the connection with the q -deformed harmonic oscillator, let us define

$$D = \frac{1}{1-q} + \frac{1}{\sqrt{1-q}} \hat{a} \quad (99)$$

$$E = \frac{1}{1-q} + \frac{1}{\sqrt{1-q}} \hat{a}^\dagger \quad (100)$$

One finds that the algebraic rules (89–91) reduce to

$$\hat{a}\hat{a}^\dagger - q\hat{a}^\dagger\hat{a} = \mathbb{1} \quad (101)$$

$$\langle W | \hat{a}^\dagger = \frac{w}{\sqrt{1-q}} \langle W | \quad \text{where} \quad w = \frac{1-q}{\alpha} - 1 \quad (102)$$

$$\hat{a} | V \rangle = \frac{v}{\sqrt{1-q}} | V \rangle \quad \text{where} \quad v = \frac{1-q}{\beta} - 1. \quad (103)$$

Thus D and E are related to the q -bosonic operators discussed in Section 4; such a relationship was first pointed out in [49]. Also we see that $\langle W|$ and $|V\rangle$ are eigenvectors of the q -bosonic operators. Such eigenvectors are known as coherent states (see exercise 3). In the oscillator's "energy" eigenbasis $\{|n\rangle\}$ (61) one can check that they have components

$$\langle n|V\rangle = \frac{v^n}{\sqrt{(q;q)_n}} \quad \langle W|n\rangle = \frac{w^n}{\sqrt{(q;q)_n}}. \quad (104)$$

For the moment we consider $v < 1$, $w < 1$ so that the vectors (104) are normalisable.

We introduced earlier a matrix C which appears in the expressions for the mean particle density and current. We now see that this matrix can be written as a linear combination of the identity $\mathbb{1}$ and the "position" operator $\hat{x} = \hat{a} + \hat{a}^\dagger$:

$$C = D + E = \frac{2}{1-q} \mathbb{1} + \frac{1}{\sqrt{1-q}} \hat{x}. \quad (105)$$

As we saw in Section 4 the eigenstates of the oscillator in the co-ordinate representation are continuous q -Hermite polynomials. Clearly, the eigenvectors of C are the same as those for \hat{x} and therefore knowledge of them permits diagonalisation of C .

Let us illustrate how to apply the procedure to obtain an expression for the normalisation Z_N when $q < 1$. First we insert a complete set of states into the expression for the normalisation (88):

$$Z_N = \int_0^\pi d\theta \nu(\theta) \langle W|C^N|\theta\rangle \langle \theta|V\rangle. \quad (106)$$

By design, the matrix C is acting on its eigenvectors, so using (105) and

$$\hat{x}|\theta\rangle = \frac{2 \cos \theta}{\sqrt{1-q}} |\theta\rangle \quad (107)$$

we obtain

$$Z_N = \int_0^\pi d\theta \nu(\theta) \langle W|\theta\rangle \left(\frac{2(\cos \theta + 1)}{1-q} \right)^N \langle \theta|V\rangle. \quad (108)$$

Now we know the form of $\langle W|$ and $|V\rangle$ in the $\{|n\rangle\}$ basis (104). Therefore we insert a complete set of the basis vectors in (108) to find

$$\langle \theta|V\rangle = \sum_{n=0}^{\infty} \langle \theta|n\rangle \langle n|V\rangle = \sum_{n=0}^{\infty} \frac{v^n}{\sqrt{(q;q)_n}} \langle \theta|n\rangle. \quad (109)$$

Observe that the final sum in this equation is nothing but (73), the generating function of the q -Hermite polynomials! Thus, when $|v| < 1$ and $|w| < 1$, we may write

$$\langle \theta | V \rangle = G(\theta, v) \quad \langle W | \theta \rangle = G(\theta, w) \quad (110)$$

where $G(\theta, \lambda)$ is given by expression (79).

Putting all this together, we arrive at an exact integral form for the normalisation

$$Z_N = \left(\frac{1}{1-q} \right)^N \int_0^\pi d\theta \nu(\theta) [2(1 + \cos \theta)]^N G(\theta, w) G(\theta, v) \quad (111)$$

which, written out more fully and using the notation (76), reads

$$Z_N = \frac{(q; q)_\infty}{2\pi} \left(\frac{1}{1-q} \right)^N \int_0^\pi d\theta [2(1 + \cos \theta)]^N \frac{(e^{2i\theta}, e^{-2i\theta}; q)_\infty}{(ve^{i\theta}, ve^{-i\theta}, we^{i\theta}, we^{-i\theta}; q)_\infty}. \quad (112)$$

When $|v| > 1$ or $|w| > 1$ equation (111) is not well-defined because $G(\theta, \lambda)$ does not converge when $|\lambda| > 1$. Rather than finding a representation of the quadratic algebra (89–91) that does not suffer from this problem, one can simply analytically continue the integral (112) to obtain Z_N when $|v|$ or $|w|$ takes on a value greater than one. Since a contour integral is defined by the residues it contains, to analytically continue the integral one simply has to follow the poles of the integrand as they move in and out of the original integration contour (see exercise 4).

One can also apply the procedure of the previous section to find an integral representation of the normalisation for the case of $q > 1$. The only difference is that we must use the $q > 1$ polynomials. It turns out that this amounts to substituting $\cos \theta$ by $i \sinh u$ with the limits on u now running from $-\infty$ to $+\infty$ and using the weight function (86)

$$Z_N = \left(\frac{1}{1-q} \right)^N \int_{-\infty}^{\infty} du \nu(u) [2(1 + i \sinh u)]^N G(u, w) G(u, v). \quad (113)$$

It is possible to derive an alternative expression for Z_N which takes the form of a finite sum rather than an integral and is valid for *all* values of the model parameters. Such an expression implies the solution of the combinatorial problem of reordering operators D, E under the rule (89). In [51] the formula (eq. 55 in that paper) was derived by explicitly evaluating the integral (111) using further properties of q -Hermite polynomials and their generating functions.

5.3 Phase diagram

The phase diagram for the partially asymmetric exclusion process is now obtained by calculating the current through the relation $J = Z_{N-1}/Z_N$ and the above exact expressions for the normalisation Z_N .

For the case of *forward bias* ($q < 1$) in which particle hops are biased from the left boundary (where particles are inserted) to the right boundary (where they are removed) one expects a nonvanishing current in the thermodynamic limit $N \rightarrow \infty$. This is calculated by applying the saddle-point method to the integral (112)—see exercise 4. It turns out that for large N

$$\langle W|C^N|V\rangle \sim a^N N^{-\gamma} \quad (114)$$

Then in the thermodynamic limit $J \rightarrow 1/a$. Phase transitions arise from different asymptotic forms of the current due to the analytic continuation (see exercise 4) for the integral (112). Ultimately one finds the expressions presented in Table 1 and thence the phase diagram shown in Figure 5.

Note that the current as given by (96) is a ratio of two partition functions of size $N - 1$ and N . In equilibrium statistical mechanics (in the large N limit) this ratio is equivalent to the fugacity z (within the grand canonical ensemble). Recalling that $z = e^\mu$ and the chemical potential μ is equivalent to the Gibbs free energy per particle, gives credence to our claim in section 2.1.4 that the current J acts as a free energy for the system.

We note that this phase diagram has a very similar form to that of Figure 3 which applied for the special case of total asymmetry $q = 0$. That is, one finds the same three phases, namely a (i) high density, (ii) low density and (iii) maximal current phase. As discussed in Section 2.1 the transition between the low and high density phases (i) and (ii) is first order and those to the maximal current phase (iii) are second order. Note from Table 1 that, for example,

Phase	Region	Current J
(i)	$\beta \leq \frac{1-q}{2}$, $\alpha \geq \beta$	$\frac{\beta(1-q-\beta)}{1-q}$
(ii)	$\alpha \leq \frac{1-q}{2}$, $\beta \geq \alpha$	$\frac{\alpha(1-q-\alpha)}{1-q}$
(iii)	$\alpha \geq \frac{1-q}{2}$, $\beta \geq \frac{1-q}{2}$	$\frac{1-q}{4}$

Table 1

The $N \rightarrow \infty$ forms of the particle current in the forward biased phases.

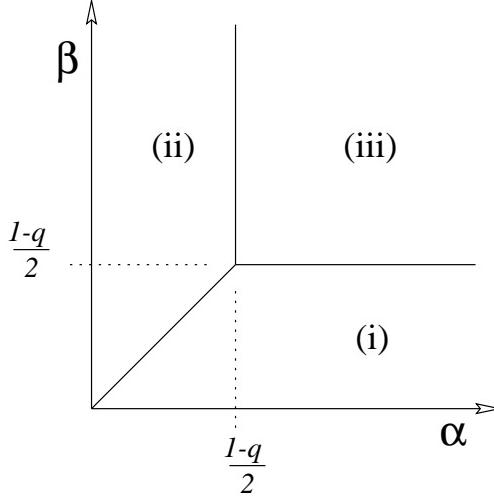


Fig. 5. The phase diagram for the current in the forward-bias regime of the PASEP. first derivative of the current is discontinuous at the transition between the low and high density phases.

Similar methods can be used to find the density profiles in the PASEP: the details of the calculations and results are presented in [52]. It turns out that the low- and high-density phases subdivide into three subphases for nonzero q less than one [52]. In each of the low density subphases, the bulk density is $\rho = \alpha/(1 - q)$; however what distinguishes the subphases is that the decay of the density profile from the right boundary takes a different form in each. The same is true of high-density phase, except that $\rho = (1 - \beta)/(1 - q)$ and that the density decay is at the left boundary.

Exercise 4: Evaluation of the current in the PASEP with $q < 1$

Show that the integral representation of the normalisation for $q < 1$, equation (112), can be recast as a contour integral

$$Z_N = \oint_C dz \exp(Nh(z))g(z) \quad (\text{E4.1})$$

where C is the unit circle centred on the origin,

$$h(z) = \ln(2 + z + z^{-1}) - \ln(1 - q) \quad \text{and} \quad g(z) = \frac{1}{4\pi iz} \frac{(q, z^2, z^{-2}; q)_\infty}{(vz, v/z, wz, w/z; q)_\infty}.$$

The large number of singularities in the integrand at the origin makes this a difficult integral to evaluate exactly using, *e.g.*, the residue theorem. Instead, we shall use this contour integral to obtain the currents in the PASEP for large system size.

First, we will apply the saddle-point method to the above integral which is valid for the range $|v| < 1, |w| < 1$. The idea is to deform the contour of integration such that it passes through a saddle point in $\text{Re}[h(z)]$ along the path of steepest descent (this

is also the line where $\text{Im}[h(z)] = \text{const}$). Show that this saddle point is at $z_0 = 1$ and that the path of steepest descent (at least near z_0) is parallel to the imaginary axis. Also, show that $g(z_0) = g'(z_0) = 0$.

Insert Taylor expansions of $h(z)$ and $g(z)$ (to second order) about the saddle point z_0 into (E4.1) to obtain

$$Z_N = \exp(Nh(z_0)) \oint_C dz \exp\left(-\frac{1}{2}Nh''(z_0)(z - z_0)^2\right) \frac{g''(z_0)}{2}(z - z_0)^2.$$

You should now convince yourself that the deformation of the integration contour to pass through z_0 along the path of steepest descent in $\text{Re}[h(z)]$ is equivalent to making the substitution $z = z_0 + ix$ with x running from $-\infty$ to $+\infty$. Hence show that the resulting Gaussian integral will give rise to an expression of the form

$$Z_N \sim K_1 \exp(Nh(z_0)) N^{-3/2}.$$

Note: to save time, do not evaluate the constant K_1 (although you may like to check that it is real and positive).

Now show that the current in the PASEP for $|v| < 1$, $|w| < 1$ and large N behaves as

$$J = \frac{Z_{N-1}}{Z_N} \sim \frac{1}{\exp h(z_0)} = \frac{1-q}{4}.$$

There now remains the question of what to do when one of the control parameters, say v , has a magnitude greater than 1. When $|v| < 1$, the contour C encloses the poles of $g(z)$ at $z = v, qv, q^2v, \dots$ but excludes those at $z = 1/v, q/v, q^2/v, \dots$. As v is increased, the pole at $z = v$ moves outside C and that at $z = 1/v$ moves inside. To obtain the analytic continuation of Z_N , one must add to the saddle-point expression for the integral over C above the residue at $z = v$ and subtract that at $z = 1/v$. Show that this yields

$$Z_N \sim K_1 \exp(Nh(z_0)) N^{-3/2} + K_2 \exp(Nh(v)).$$

Again try to avoid explicitly calculating the positive constant K_2 . Verify that $h(v) > h(z_0)$ and thus that, for sufficiently large N , $Z_N \sim K_2 \exp(Nh(v))$. Hence show that for $1 < v < 1/q$

$$J = \frac{Z_{N-1}}{Z_N} \sim \frac{1}{\exp h(v)} = \frac{\beta(1-q-\beta)}{1-q}.$$

Now convince yourself that as v is increased yet further, the contribution from the additional poles that have entered/exited the unit circle is smaller than that from those at $z = v, 1/v$. Consider also the effect of increasing w to a value less than v and show that when $w > v, w > 1$

$$J \sim \frac{1}{\exp h(w)} = \frac{\alpha(1-q-\alpha)}{1-q}.$$

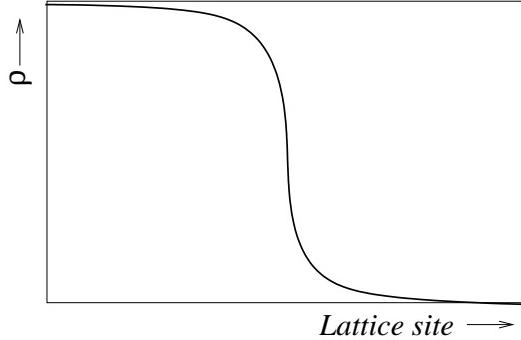


Fig. 6. Proposed form of the density profile in the reverse-bias regime of the PASEP.

Finally, use the information learned from this analysis to construct the phase diagram (Figure 5) for the current in the α - β plane.

For $q > 1$ one has a reverse bias regime [51] where the boundary conditions force a current through the system against the direction of the reverse bias. This gives rise to a new phase in which the current decreases exponentially with the length of the system as $J \sim q^{-N/2}$. This phase is of interest in the context of ‘backbias dynamics’ [53,54] where, for example, a fluid in a permeable medium has to traverse a pore oriented against the direction of gravity.

One can predict the form of the density profile in the reverse bias regime as follows. We expect a high-density region at the left edge of the lattice, towards which the particles are biased but cannot escape, and a low-density region at the right edge of the lattice. Thus the density profile is a Fermi-like function as illustrated in Figure 6. In order that the profile is stationary the typical time for a particle to diffuse (against the bias) from the edge of the high-density region to the right boundary must be equal to the typical time of a hole to diffuse from the edge of the low-density region to the left boundary. Since the diffusion rates of both particles and holes are the same, the boundary between the high- and low-density regions must be in the centre of the lattice, as illustrated in Figure 6.

5.4 Generalisations

Here we give a brief overview of other related exclusion processes. Firstly the features of the phase diagram for $q < 1$ (Figure 5) appear robust for stochastic one-dimensional driven systems and can be predicted from considerations of domain wall dynamics [55,56]. This has been confirmed through the exact solution of the open boundary system with fully parallel dynamics [57,58].

However when the bulk dynamics become deterministic the maximal current phase is lost.

For the case of symmetric exclusion $q = 1$ (no bulk drive) one does not have phase transitions; the current is easy to calculate and decays linearly with system size [59–61]. Intuitively one can understand this as diffusion between two particle reservoirs of different density. The diffusion current will be proportional to the concentration gradient which decreases as $1/N$. Thus although the bulk dynamics is symmetric the boundary conditions force a weak current of particle through the system.

For $q = 1$ a recent work [62] has determined the probability of observing a particular coarse-grained density profile $\rho(x)$. In an equilibrium system, this probability is given by $\exp(-N\mathcal{F}[\rho])$ in which $\mathcal{F}[\rho]$ is a local functional that expresses the free energy difference between the equilibrium profile and ρ . From the matrix product approach a form for a functional that plays a similar role in the symmetric exclusion process was found in [62] and is shown to be *nonlocal*. For the particular boundary conditions where the dynamics satisfy detailed balance, $\mathcal{F}[\rho]$ reduces to the free energy functional known from equilibrium statistical physics and so the nonlocal functional would seem to generalise a well-known equilibrium concept.

An interesting kind of boundary-induced phase transition, manifesting spontaneous symmetry breaking, is found when the asymmetric exclusion process is generalised to two oppositely moving species of particle: one species is injected at the left, moves rightwards and exits at the right; the other species is injected at the right, moves leftwards and exits at the left [63]. Intuitively one can picture the system as a narrow road bridge: cars moving in opposite directions can pass each other but cannot occupy the same space. The model has a left-right symmetry when the injection rates and exit rates for the two species of particles are symmetric. However for low exit rates (β) this symmetry is broken and the lattice is dominated by one of the species at any given time. This implies that the short time averages of currents and bulk densities of the two species of particles are no longer equal. Over longer times the system flips between the two symmetry-related states. In the $\beta \rightarrow 0$ limit the mean flip time between the two states has been calculated analytically and shown to diverge exponentially with system size [64]. Thus the ‘bridge’ model provided a first example of spontaneous symmetry breaking in a one dimensional system.

In the models discussed so far the open boundaries can be thought of as inhomogeneities where the order parameter (particle density) is not conserved. Inhomogeneities which conserve the order parameter can be considered on a periodic system. Indeed a single defect bond on the lattice (through which particles hop more slowly) is sufficient to cause the system to separate into two macroscopic regions of different densities [65]: a high density region which

can be thought of as a traffic jam behind the defect and a low density region in front of the defect. Here the presence of the drive appears necessary for the defect to induce the phase separation. Moving defects (*i.e.* particles with dynamics different from that of the others) have also been considered and exact solutions obtained [66–69]. For the simple case of a slowly moving particle the phenomenon of a queue of particles forming behind it has been shown to be analogous to Bose condensation [70,71].

6 Stochastic Ballistic Annihilation and Coalescence

In Section 2.2 we introduced two reaction systems, namely annihilation ($A + A \rightarrow \emptyset$) and coalescence ($A + A \rightarrow A$). As noted in Section 2.2, it is well known that annihilation and coalescence reactions are equivalent when the reactant motion is diffusive [14,15] and hence lead to the same $t^{-1/2}$ density decay in one dimension.

We now consider in detail the distinct case of ballistic reactant motion by which it is meant that particles move with some fixed velocity. We study a class of models that comprise an arbitrary combination of annihilation and coalescence of particles with two (conserved) velocities and stochastic reaction dynamics and which was solved in [73]. As we shall see, an exact solution is possible by virtue of a matrix product method in which the matrices involved can be written in terms of the raising and lowering operators of the q -deformed harmonic oscillator. A related, but distinct, ballistic reaction model (not contained within the class discussed here) had also revealed a connection between ballistic reaction systems and q -deformed operator algebras [74].

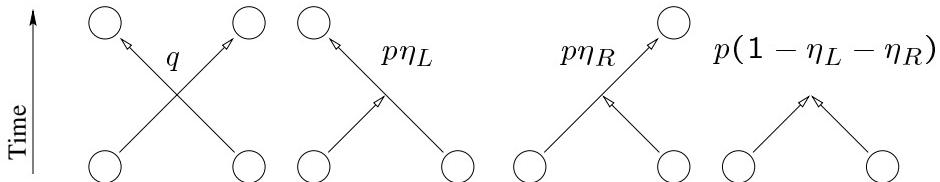


Fig. 7. The possible reactions and their probabilities.

We now define the class of models to be considered. At time $t = 0$ reactants are placed randomly on a line. Each particle is assigned a velocity $+c$ (right-moving) or $-c$ (left-moving) with probability f_R and $f_L = 1 - f_R$ respectively. Particles move ballistically until two collide, at which point one of four outcomes follows, see Figure 7: the particles pass through each other with probability q ; the particles coalesce into a left (right) moving particle with probability $p\eta_L$ ($p\eta_R$); the particles annihilate with probability $p(1 - \eta_L - \eta_R)$. Here $p = 1 - q$ is the probability that some reaction occurs.

As an example of an application of this model consider the identification of

right- and left-moving particles with the edges of terraces as illustrated in Figure 8. If new particles are added to the system in such a way that they only stick to the sides, and the rate of particle addition is taken to infinity, one obtains ballistic motion of terrace edges. When two edges meet, a terrace is completed which corresponds to annihilation of approaching particles. Hence the relevant parameters of the general annihilation coalescence model are $\eta_L = \eta_R = 0$. The scattering reaction, which occurs with rate q , corresponds to the possibility of a new terrace being formed when two edges meet.

The case of deterministic annihilation $q = \eta_L = \eta_R = 0$ was studied by Elskens and Frisch [20]. Here particles always annihilate on contact. This case was found to exhibit a density decay that depends on time as $t^{-1/2}$, but only if the initial densities of the two particle species (left- and right-moving) are the same. In the following analysis of the more general class of reaction systems, we find that such a result persists if two ‘effective’ initial densities (to be defined below) are equal. Furthermore, we will see that the introduction of stochasticity into the reaction dynamics *i.e.* the parameter q , induces a transition in the density decay form.

Our aim is to calculate the density decay. To do this we shall consider without loss of generality a right moving test particle as illustrated in figure 9. We define $P_S^{(R)}(t)$ as the probability that the test particle survives up to a time t respectively. From figure 9 one can see that the initial spacing of the particles on the line does not affect the *sequence* of possible reactions for any given particle, in particular for the test particle (we return to this point later). Also note that after a given time t , the test particle may only have interacted with the N particles initially placed within a distance $X = 2ct$ (and to the right) of the chosen particle. These two facts imply that the survival probability can be expressed in terms of two independent functions. The first is $G(N; X)$, the probability that initially there were exactly N particles in a region of size $X = 2ct$. The second is $F(N)$, the probability that the test particle survives reactions with the N particles initially to its right, and depends only on the

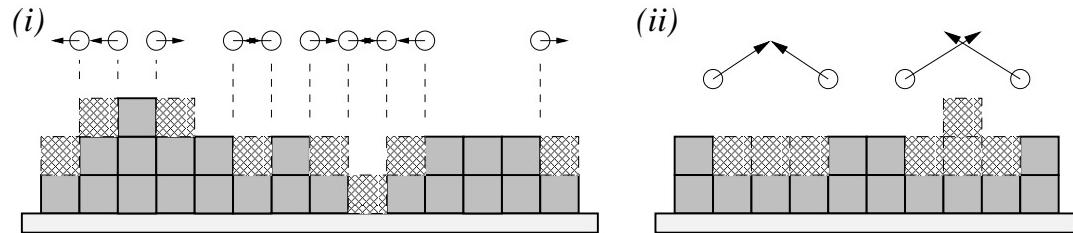


Fig. 8. (i) Mapping of a surface growth model to a particle reaction system through the identification of upward and downward steps to left- and right-moving particles. Addition of new particles that stick only to the sides of the surface cause the particles to move. (ii) The correspondence of particle annihilation and scattering to the elimination and nucleation of a terrace respectively.

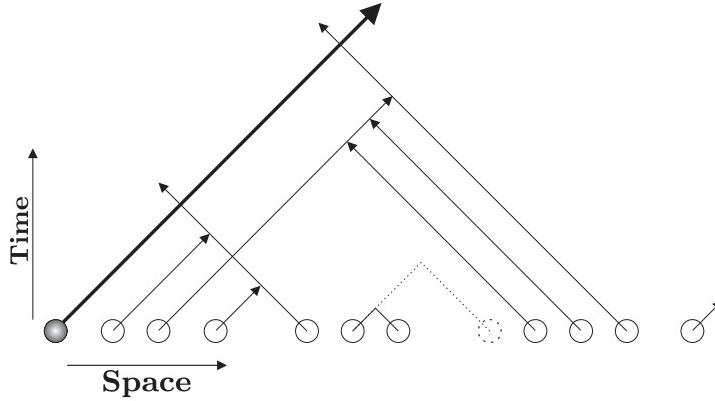


Fig. 9. A configuration and set of trajectories and reactions for a test particle (shaded and bold line) encountering a string of $N = 10$ particles. Note how changing the spacing between, for example, the fifth and sixth particles (indicated by dotted lines) alters the time sequence of the reactions but not the final survival probability.

sequence of the N particles. Explicitly,

$$P_S^{(R)}(X) = \sum_{N=0}^{\infty} G(N; X) F(N) . \quad (115)$$

Thus the problem is reduced to two separate combinatorial problems of calculating $G(N; X)$ and $F(N)$. Note that the choice of $G(N; X)$ allows one to consider a model defined on a lattice or on the real line. In the present work we assume particles are initially placed on a line with nearest-neighbour distances chosen independently from an exponential distribution with unit mean. Then we can use a well-known result [29]

$$G(N; X) = X^N e^{-X} / N! . \quad (116)$$

We now show that the second problem (calculation of $F(N)$) can be formulated within a matrix product approach.

As an example consider a test particle encountering the string of reactants depicted in Figure 9. We claim that the probability of the test particle surviving through this string may be written as

$$\langle W | R R R L R L L L L R | V \rangle \quad (117)$$

where R, L are matrices and $\langle W |, |V \rangle$ vectors with scalar product $\langle W | V \rangle = 1$. Thus we write, in order, a matrix R (L) for each right (left) moving particle in the initial string.

The conditions for an expression such as (117) to hold for an arbitrary string are, in fact, rather intuitive

$$RL = qLR + p(\eta_L L + \eta_R R + [1 - \eta_L - \eta_R]) \quad (118)$$

$$\langle W|L = \langle W|(q + p\eta_R) \quad (119)$$

$$R|V\rangle = |V\rangle . \quad (120)$$

The condition (118) just echoes the reactions that occur in Figure 7 *i.e.* after an interaction between a right-moving and left-moving particle there are four possible outcomes (see Figure 7) corresponding to the four terms on the right hand side of (118) with probabilities given by the respective coefficients. Using (118), any initial matrix product such as (117) can be reduced to a sum of terms of the form $\langle W|L^s R^t|V\rangle$ corresponding to all possible final states ensuing from the initial string and with coefficients equal to the probabilities of each final state. These final states give the possible sequences of particles that the right-moving test particle will encounter. The test particle will survive such a final state and pass through the s left-moving particles with probability $(q + p\eta_R)^s$. The condition (120) ensures that this probability is obtained for each possible final state *i.e.*

$$\langle W|L^s R^t|V\rangle = (q + p\eta_R)^s \langle W|R^t|V\rangle . \quad (121)$$

Finally the condition (119), along with $\langle W|V\rangle = 1$, ensures that once a right-moving particle passes through all the left-moving particles in the string it no longer plays a role. Thus (121) becomes

$$\langle W|L^s R^t|V\rangle = (q + p\eta_R)^s . \quad (122)$$

Note that the reason for a matrix product formulation is different from the PASEP. There the steady state probability of any configuration, for arbitrary system size, could be written as a matrix product. Here the probability of a particle surviving some arbitrary sequence of particles can be written as a matrix product.

The above approach relies on an important property of the system which is invariance of a reaction sequence with respect to changes of initial particle spacings. To understand this, consider again Figure 9. By altering the initial spacings of the particles, the absolute times at which trajectories intersect and reactions may occur (if the reactants have survived) may be altered. For example, by increasing the spacing between the fifth and sixth particles, the trajectories of the third and fourth particles can be made to intersect first. However as we have already seen, for any particle, the *order* of intersections it encounters does not change and so the final states and probabilities are invariant. This invariance is manifested in the matrix product by the fact that the order in which we use the reduction rule (118) is unimportant *i.e.* matrix multiplication is associative. Thus, it is the invariance with respect to initial spacings that allows the system to be solved by using a product of matrices.

We now proceed to evaluate $F(N)$. Averaging (117) over all initial strings of length N , recalling that f_R and f_L are the probabilities that a particle is assigned velocity $+c, -c$ respectively, yields

$$F(N) = \langle W | (f_L L + f_R R)^N | V \rangle . \quad (123)$$

To evaluate $F(N)$ we first write

$$R = \frac{\sqrt{f_R^* f_L^*}}{f_R} \hat{a} + \eta_L \quad \text{and} \quad L = \frac{\sqrt{f_R^* f_L^*}}{f_L} \hat{a}^\dagger + \eta_R . \quad (124)$$

In these equations we have introduced two new parameters

$$f_R^* = f_R(1 - \eta_L) \quad \text{and} \quad f_L^* = f_L(1 - \eta_R) \quad (125)$$

which we call effective initial particle densities and whose ratio

$$\chi = \frac{f_R^*}{f_L^*} \quad (126)$$

turns out to be an important parameter of the model.

One can verify from (118–120) that \hat{a}, \hat{a}^\dagger satisfy a q -deformed harmonic oscillator algebra

$$\hat{a}\hat{a}^\dagger - q\hat{a}^\dagger\hat{a} = 1 - q \quad (127)$$

$$\langle W | a^\dagger = \langle W | q / \sqrt{\chi} \quad (128)$$

$$a | V \rangle = \sqrt{\chi} | V \rangle . \quad (129)$$

Thus (123) can be written as

$$F(N) = \langle W | \left[\sqrt{f_R^* f_L^*} (\hat{a} + \hat{a}^\dagger) + 1 - f_L^* - f_R^* \right]^N | V \rangle . \quad (130)$$

The vectors $\langle W |$ and $| V \rangle$ are eigenvectors of \hat{a}^\dagger, \hat{a} , and as in Section 5, they can be explicitly calculated.

At this point one can see that we have precisely the same mathematical structure as we did when solving for the steady state of the PASEP—compare (127–129) with (101–103). We just need to carry out the same procedure of diagonalising a matrix that is linear combination of the identity operator and the position operator of a q -deformed harmonic oscillator. Rather than repeat the details here we go directly to a discussion of the phase diagram.

Exercise 5: Deterministic ballistic annihilation and random walks

The Elskens-Frisch model [20] of deterministic ballistic annihilation is a special case of the stochastic model described above that has the parameters $q = \eta_L = \eta_R = 0$. For the case where particles are initially placed on all sites of a lattice with equal probability of right- and left-moving particles, write down all possible initial conditions that would allow a right-moving test particle to survive through one, two and three sites. Hence relate the survival probability of the test particle after N sites to the probability of a random walker not returning to the origin after $N + 1$ steps. Hint: devise a criterion for the survival of the test particle that involves the relative number of left- and right-moving particles for a given initial condition.

Construct the matrices R and L and the vectors $\langle W |$ and $| V \rangle$ and explain how the resulting expression for $F(N)$ (with $f_L = f_R = \frac{1}{2}$) is related to the random walk problem.

6.1 Phase diagram

We consider the long-time density decay $\varrho(t)$ which is obtained from the survival probabilities $P_S^{(R)}(t)$, $P_S^{(L)}(t)$ for right and left moving test particles through

$$\varrho(t) = f_R P_S^{(R)}(t) + f_L P_S^{(L)}(t) . \quad (131)$$

($P_S^{(L)}(t)$ can be deduced from $P_S^{(R)}(t)$ through the left-right symmetry of the model.)

The matrix product calculation for $F(N)$ implies that the density decays as

$$\varrho(t) = \varrho_\infty + \Delta(t) . \quad (132)$$

In this equation $\varrho_\infty = f_L(1 - \chi)$ is the fraction of particles remaining once no more reactions are possible (*i.e.* all particles moving in the same direction). We now list the results the residual density ϱ_∞ when $\chi < 1$. (Results for $\chi > 1$ one be deduced using the left-right symmetry of the model.)

For $\chi < q^2$

$$\Delta(t) = f_R \left(1 - \frac{f_R^*}{q^2 f_L^*} \right) \exp \left[-2 (1 - q) (f_L^* - f_R^*/q) ct \right]$$

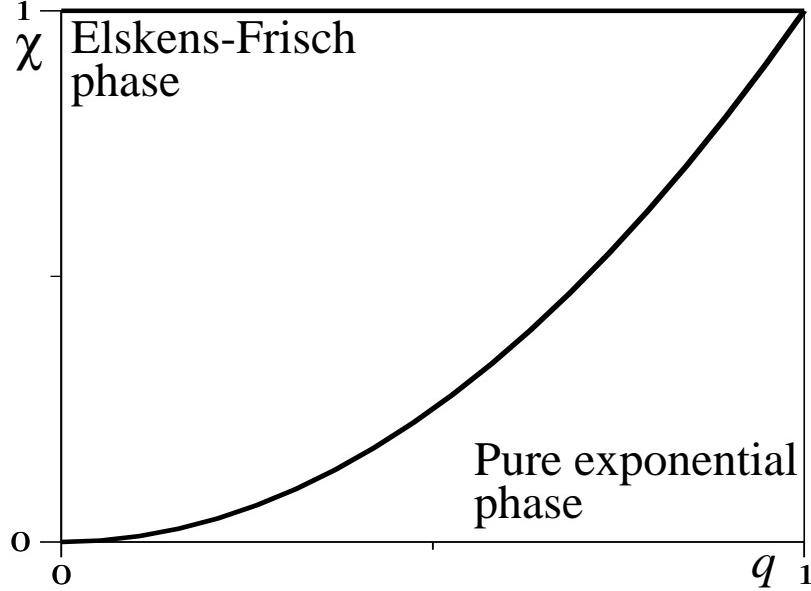


Fig. 10. Phase diagram for the model of stochastic ballistic annihilation and coalescence. The density decay form depends on the ratio of effective densities χ and the stochasticity parameter q .

For $\chi = q^2$

$$\Delta(t) = \frac{f_R}{\sqrt{2\pi}} \left(\frac{1}{f_L^* f_R^*} \right)^{\frac{1}{4}} \frac{\exp \left[-2(\sqrt{f_L^*} - \sqrt{f_R^*})^2 ct \right]}{(ct)^{1/2}}$$

For $q^2 < \chi < 1$

$$\begin{aligned} \Delta(t) = & \frac{(q; q)_\infty^4}{4\sqrt{2\pi}(q\sqrt{\chi}, q/\sqrt{\chi}; q)_\infty^2} \\ & \times \left(\frac{1}{f_L^* f_R^*} \right)^{\frac{3}{4}} \frac{f_L f_R^* + f_R f_L^*}{(\sqrt{f_L^*} - \sqrt{f_R^*})^2} \frac{\exp \left[-2(\sqrt{f_L^*} - \sqrt{f_R^*})^2 ct \right]}{(ct)^{3/2}} \end{aligned}$$

For $\chi = 1$

$$\Delta(t) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{f_L^* f_R^*} \right)^{\frac{1}{4}} \left(\frac{1}{ct} \right)^{\frac{1}{2}}$$

We now consider the phase diagram—figure 10. This is spanned by the values of χ (the ratio of effective densities $\chi = f_R^*/f_L^*$) and q (the stochasticity parameter): χ parameterises all information concerning the asymmetry between the right and left moving particles whereas q parameterises the level of stochasticity. Thus there is universality of ballistic annihilation and coalescence: for a generic choice of η_R , η_L defining a particular annihilation-coalescence model, the same four decay regimes are found by varying the initial densities or stochasticity parameter q . In this way the universality can be considered as a ‘law of corresponding states’.

The line $\chi = 1$ (equal effective densities) is non-generic since a single, power law, decay regime is found. The decay does not depend on the stochasticity q . This special line was found by Elskens and Frisch [20] for the case of deterministic annihilation ($\eta_L = \eta_R = q = 0$) and we have shown that this special line is present for all combinations of annihilation and coalescence. This phase can be understood through the picture of [20]. Density fluctuations in the initial conditions lead to trains of left- and right-moving particles: in a length $\sim t$ the excess particle number is $\sim t^{1/2}$ which yields the $t^{-1/2}$ density decay. At long times, the train size is large and so a particle in one train encounters many particles in the other and will eventually react making the parameter q irrelevant.

The second phase found in [20] (labelled the Elskens-Frisch phase in the diagram) is seen to persist for nonzero q and in this phase the two particle species decay at equal rates. The two new phases that arise in the full model for $\chi \leq q^2$ (*i.e.* as a consequence of randomness in the reaction dynamics) have the contrasting property that two particle species decay at *unequal* rates leaving a non-zero population of left-moving particles. A simple example of non-equal decays is the case $\eta_R = 0, \eta_L = 1$ ($\chi = 0$). Then left-moving particles do not decay but simply absorb the right-moving particles with probability $1 - q$ giving $\varrho = f_R e^{-2(1-q)f_L c t}$. Our results show that, in general, increasing q leads to a non-trivial transition at $\chi = q^2$ to a regime where the two species have different decay forms.

7 Conclusion

In these lectures we have tried to give a flavour of the collective phenomena exhibited by simple low-dimensional systems with stochastic dynamics. Specifically we have seen that the partially asymmetric exclusion process exhibits a number of phase transitions (of both first and second order) and long-range correlations even in one dimension. We have also shown how similar mathematical techniques can be applied in the distinct context of a particle reaction system to obtain an exact solution.

We hope that the reader with a background in equilibrium statistical physics is pleasantly surprised by the diversity of phenomena that emerge in low-dimensional nonequilibrium systems. We have also endeavoured to illustrate how novel analytical techniques are being developed for these systems. Through the inclusion of background material and the exercises, we hope also to have inspired confidence in the reader to approach the literature and make an active contribution to this fertile field.

Acknowledgments: We would like to thank our collaborators F. Colaiori, F.

Essler and Y. Kafri with whom the work of section 5 and section 6 was carried out and also M. J. E. Richardson who contributed to the early development of that work.

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